



**VISTEC**  
VIDYASIRIMEDHI  
INSTITUTE OF SCIENCE AND TECHNOLOGY



**20**  
ANNIVERSARY  
NANOTEC  
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# NANO THAILAND 2023

The 8<sup>th</sup> Thailand International  
Nanotechnology Conference

**“Nanotechnology for  
Sustainable World”**

## Abstract Book

**November 29- December 1, 2023**  
**Dusit Thani Pattaya Hotel,**  
**Chon Buri, Thailand**

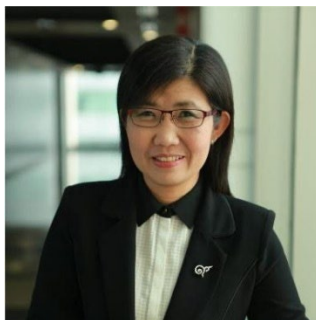
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<https://www.nano-thailand.com/> / [nanothailand2023@gmail.com](mailto:nanothailand2023@gmail.com)

## Welcome Message

From the Nanotechnology Association of Thailand and National Nanotechnology Center  
(NANOTEC)



**Dr. Wannee Chinsirikul**

Executive Director of the National Nanotechnology Center (NANOTEC) and President of the  
Nanotechnology Association of Thailand

On behalf of the Nanotechnology Association of Thailand, it is my great pleasure and privilege to extend a warm invitation to you all for participating the 8th Thailand International Nanotechnology Conference (NanoThailand 2023), which will be held during 29 November – 1 December 2023 at Pattaya, Chonburi, Thailand. I would like to take this opportunity to express my sincere appreciation to Vidyasirimedhi Institute of Science and Technology (VISTEC), National Nanotechnology Center (NANOTEC) and the Nanotechnology Association of Thailand to organize this conference.

The theme of the conference is “Nanotechnology for Sustainable World”. The objectives are to apply nanoscience and nanotechnology for a better life and well-being to create a platform for knowledge exchange to further advance technological areas, and to exhibit the latest innovations to the industries. At present, we are collaborating in areas such as e-science, renewable energy and the development of novel drugs to combat a range of infectious diseases. Therefore, Science, Technology, Innovation and technology know-how cooperation among peers are very important. NanoThailand 2023 will provide a platform for experienced researchers in nanotechnology and practitioners from both academics, as well as industry to meet and share cutting-edge development in the field. In order to meet the objectives of the conference, the world renowned speakers, and researchers are invited to present the advancement of nanoscience and to update trend of the World’s nanotechnology of their expertise.

I would like to welcome all participants, and to our overseas friends, please enjoy the breath and depth of Science and Technology at the upcoming NanoThailand 2023 (29 November – 1 December 2023) in the vibrant east coastal city of Thailand where you could take times to also absorb many attractive sites there is to offer in Pattaya.



## Welcome Message

Form Vidyasirimedhi Institute of Science and Technology (VISTEC)



**Professor Dr. Pimchai Chaiyen**

President of Vidyasirimedhi Institute of Science and Technology (VISTEC)

On behalf of Vidyasirimedhi Institute of Science and Technology (VISTEC), it is my great pleasure to welcome you all to the 8<sup>th</sup> Thailand International Nanotechnology Conference (NanoThailand 2023), being held between 29 November – 1 December 2023 at Dusit Thani Hotel, Pattaya, Thailand. VISTEC is proud to be a co-host of this conference.

The conference's theme is "Nanotechnology for Sustainable World" and its objectives are to apply nanotechnology in various fields to contribute to sustainable development. The conference will create a platform for technological knowledge exchange, and to share the latest progress in research and innovations towards a sustainable world. We are expecting around 350 participants from more than 20 countries to attend NanoThailand 2023. The conference features 13 sessions with 2 plenary lectures, 97 keynote and invited talks, 97 oral presentations and 82 posters covering all fields of nanotechnology.

On the scientific side, VISTEC members are contributing extensively to this conference by hosting, chairing, co-chairing, and presenting in all the sessions. Together with our co-host NANOTEC, we aim to showcase advanced and innovative nanoscience and nanotechnology research conducted in Thailand. Our members are hosting and presenting in the following sessions:

- **Session 4:** Nanomaterials and Nanotechnology for Electronic/Optoelectronic Devices and Sensors,
- **Session 5:** Nanomedicine, Nanosensor and Nano-biotechnology,
- **Session 6:** Nanotechnology for Energy Storage and Management, Session 8: Nanotechnology for Catalysis and Industrial Applications,
- **Session 9:** Nanotechnology for Startups and Industrial Enterprises, and
- **Special Session 1:** Advanced Nanostructured Materials for a Global Circular Economy.

We hope that these sessions will provide all participants insights into the current state of cutting-edge research work at VISTEC.

NanoThailand 2023 will provide all participants excellent opportunities to exchange ideas, network professionally, and broaden their knowledge. We hope that you all will have fruitful meetings and enjoy activities at Dusit Thani Hotel, the City of Pattaya, EECi and VISTEC during your excursion, as well as other places you visit in Thailand. Once again, on behalf of Vidyasirimedhi Institute of Science and Technology (VISTEC), we are looking forward to welcoming you at NanoThailand 2023 in Thailand.

## NanoThailand 2023 Organizing Committee

### Executive Advisory Committee

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Dr. Panachit Kittipanya-ngam  
Dr. Pimpisut Worakajit  
Dr. Suwussa Bamrungsap  
Dr. Kantapat Chansaenpak  
Assoc. Prof. Dr. Prapasiri Pongprayoon  
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## Local Organizing Committee

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Prof. Dr. Pimchai Chaiyen      President of Vidyasirimedhi Institute of Science and  
Technology (VISTEC)

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Prof. Dr. Vinich Promarak (VISTEC)

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Chair: Dr.Kanokwan Sansanaphongpricha

Co-chair: Dr.Teerapong Yata

### Session 2: Theory and Simulation for Nanosystems

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Co-chairs: Dr.Anchalee Junkaew

Assoc. Prof.Sarana Nutanong

### Session 3: Nanosafety and Standard

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Co-chair: Dr.Sasitorn Aueviriyavit

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Co-chairs: Prof.Albert Schulte

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Dr.Suwussa Bamrungsap

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### Session 7: Nanotechnology for Environment and Agriculture

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Co-chair: Dr.Warayuth Sajomsang

### Session 8: Nanotechnology for Catalysis and Industrial Applications

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Co-chair: Assist. Prof.Sareeya Bureekaew

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Chair: Dr.Paisan Khanchaitit

Co-chair: Dr.Pichaya Pattanasattayavong

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### Session 10: Nanocharacterization & Instrumentation

Chair: Dr. Annop Klamchuen  
Co-chairs: Dr. Pinit kidkhunthod  
Dr. Kitiphat Sinthiptharakoon  
Dr. Narong Chanlek

### Session 11: [Special Session 1]: Advanced Nanostructured Materials for a Global Circular Economy

Chair: Assoc. Prof. Chularat Wattanakit  
Co-chair: Dr. Supawadee Namuangruk

### Session 12: [Special Session 2]: Symposium on Bio-based Chemicals & Fuels from Lignocellulose 2023 (Hub of Knowledge)

Chair: Dr. Bunyarat Rungtaweevoranit  
Co-chair: Dr. Chotitath Sanpitakseree

### Session 13: [Special session 3]: The 2<sup>nd</sup> Thailand Symposium on Nanopore technology

Chair: Dr. Deanpen Japrungr  
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Dr. Thidathip Wongsurawat  
Dr. Nuankanya Sathirapongsauti  
Dr. Thitikorn Boonkoom



# Chemistry and Application of Soft Porous Crystals from MOFs/PCPs

Susumu Kitagawa

*Institute for Integrated Cell-Material Sciences (iCeMS), Kyoto University*

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## Abstract

Metal-organic frameworks (MOFs) or porous coordination polymers (PCPs) possess inherent voids that allow storing, delivering, and separating substances, particularly gases. Among them, 3<sup>rd</sup> generation MOFs called flexible MOFs or soft porous crystals (SPCs),<sup>1-4</sup> exhibit a structural change from crystal to crystal in response to physical and crystalline stimuli. This feature distinguishes them from other porous materials, reminiscent of the induced fit mechanism of bioenzymes and the cooperative phenomenon of hemoglobin. In contrast to rigid materials showing a Langmuir type I isotherm, SPCs possess a sigmoidal isotherm and higher usable capacity and efficient recognition of guest species. The flexibility depends on the binding ability and mobility of unit ligands and metal ions and other factors, including the deformation of the entire framework due to the guest molecules in the pores. Strategies using ligand functionalization have been developed to investigate the properties but have mainly focused on discovering and understanding dynamic phenomena in SPCs. This trend has now shifted towards controlling the adsorption properties for practical applications. This talk provides an essential and accessible overview of the historical background of the chemistry of SPCs, their features, and outlook as 4<sup>th</sup> generation MOFs,<sup>2,3</sup> in particular, design and synthesis, dynamic structure analysis, flexibility and function, and theoretical interpretation and prediction of the mechanism, as well as their applications.<sup>5,6</sup>

1. S. Horike, S. Shimomura, and S. Kitagawa, *Nat. Chem.*, **2009**, 1, 695.
2. S. Kitagawa, *Acc. Chem. Res.*, **2017**, 50, 514.
3. S. Kraus, N. Hosono, and S. Kitagawa, *Angew. Chem. Int. Ed.*, **2020**, 59, 15325.
4. N. Behera, J. Duan, W. Jin, and S. Kitagawa, *EnergyChem*, **2021**, 3, 100067.
5. S. Horike and S. Kitagawa, *Nature Materials*, **2022**, 21, 983.
6. Y. Su, K. Otake, J.-J. Zheng, S. Horike, S. Kitagawa, C. Gu, *Nature*, **2022**, 611, 289.

*Keywords: Porous Coordination Polymer, Metal-Organic Framework, Soft Porous Crystal, Flexibility*

**Short Bio: Prof.Dr. Susumu Kitagawa**

Susumu Kitagawa obtained a Ph.D. degree from Kyoto University. He is a distinguished professor at Kyoto University Institute for Advanced Science (KUIAS) and the Institute for Integrated Cell-Material Sciences (iCeMS), at Kyoto University. He originated the science and technology of gas with porous coordination polymers (PCPs) and metal-organic frameworks (MOFs). He predicted early on the softness of PCP/MOF crystals and demonstrated that their framework changes in response to external fields to express various functions such as storage, separation, and conversion. He named these materials soft porous crystals (SPC) as a more generic term and pioneered chemistry, which is now rapidly spreading to other porous materials. He showed a clear vision for research by categorizing PCP/MOF materials as evolving from the first- to second-generation type in the early days to the third-generation in SPC and now to the fourth-generation type. He has advocated that the 21st century will be the "age of gas," where gas will be a crucial material in all areas of the environment, energy, resources, and health, and porous materials will play an important role. He received the Japan Society of Coordination Chemistry Award (2007), the Humboldt Research Award (2008), The Chemical Society of Japan Award (2009), the Thomson Reuters Citation Laureate (Chemistry) (2010), The Medal with Purple Ribbon, the Japanese Government (2011), The RSC de Gennes Prize (2013), The 10th Leo Esaki Prize (2013), Japan Academy Award (2016) and ACS Fred Basolo Medal (2016), The 58th Fujihara Award (2017), and Chemistry for the Future Solvay Prize (2017). Thomson Reuters and Clarivate Analytics Highly Cited Researcher (2014 - 2022). He is a member of the Japan Academy, a foreign member of the Royal Society (ForMemRS), an RSC fellow, and the honorary fellowship of the Council of the Chemical Research Society of India (CRSI).



# Employing nanotechnology for single-molecule biology: from nanopore protein sequencing to chromosome organization

Cees Dekker

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## Abstract

Nanotechnology offers fantastic opportunities to contribute to biology. I will present some recent examples from my lab where nanotech single-molecule tools are used to unravel the biology of cells down to the single-molecule level.

### 1. A DNA origami turbine powered by nanoscale flow [1]

We recently built artificial nanoscale turbines. We demonstrated driven rotary motion of a nanoscale DNA origami turbine which harnessed energy from a water flow generated by a static chemical or electrical potential gradient in a solid-state nanopore. The origami nanoturbine consisted of a 6-helix DNA bundle that adopted a chiral conformation upon phoretic docking onto the nanopore and subsequently displayed a sustained unidirectional rotary motion of up to 20 revolutions/s. These artificial nano-engines operate autonomously in physiological conditions, converting energy into useful mechanical work.

### 2. Nanopore-based sequential reading of peptides [2]

We recently demonstrated a nanopore-based single-molecule peptide reader capable of reliably detecting single amino-acid substitutions within individual peptides. A peptide is linked to a DNA molecule and sequentially pulled through a biological nanopore by a DNA helicase in single amino-acid steps. Stepping ion-current signals enable discrimination of single-amino-acid substitutions in single reads. Notably, we demonstrated the capability to ‘rewind’ peptide reads, obtaining indefinitely many independent reads of the same molecule, yielding an undetectably low error rate in single-amino-acid variant identification. Recently, we expanded this concept to discriminating single post-translational modifications within peptides of mixed charge. These proof-of-concept experiments constitute a promising basis for the development of a single-molecule protein sequencer.

### 3. Real-time imaging of DNA loop extrusion by condensin and cohesin SMC complexes [3]

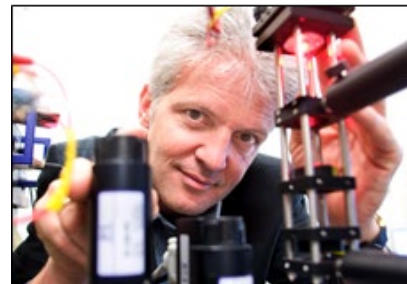
Structural Maintenance of Chromosomes (SMC) proteins like cohesin and condensin spatially organize chromosomes by extruding DNA into large loops. Using single-molecule assays, we provided unambiguous evidence for loop extrusion by directly visualizing the processive extension of DNA loops by SMCs in real-time. In recent extensions of this work, we showed how this process occurs on supercoiled DNA, that SMCs also can exhibit phase condensation, and that SMC proteins can bypass huge roadblocks of bound proteins on DNA.

References:

- [1] X. Shi et al, Nature Physics 18, 1105 (2022); X. Shi et al, Nature Nanotechnology, under review (2023).
- [2] H. Brinkerhoff et al, Science 374, 1509 (2021); I. Nova et al, Nature Biotechnology, in print (2023).
- [3] Ganji et al, Science 360, 102 (2018); Kim et al, Nature 579, 438 (2020); B. Pradhan et al, Cell Reports 41, 111491(2022).

**Short Bio: Cees Dekker**

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**Education**

1977-1983 Experimental Physics at the University of Utrecht  
1984-1988 Ph.D. in Physics from University of Utrecht; thesis "Two-dimensional spin glasses"

**Academic appointments**

1984-1988 Research assistant at the University of Utrecht  
1988-1993 Assistant professor at the University of Utrecht  
1990-1991 Visiting researcher at IBM Research, Yorktown Heights, USA  
1993-1999 Associate professor at Delft University of Technology  
1999-now Antoni van Leeuwenhoek full professor at Delft University of Technology.  
2000 Visiting researcher at Technion – Israel Institute of Technology, Haifa, Israel  
2000-now Full professor of Molecular Biophysics, Delft University of Technology  
2001-2010 Group leader of the Molecular Biophysics group  
2006-now Distinguished University Professor, Delft University of Technology  
2010-2013 Founding Chair of a new Department of Bionanoscience, TU Delft  
2010-2018 Director of the Kavli Institute of Nanoscience Delft  
2015-2020 Royal Academy Professor of the Royal Netherlands Academy of Arts and Sciences (KNAW)

**Research overview**

**2020-now** Genome-in-a-box: building a chromosome from the bottom up. To figure how the nanoscale local interactions of DNA and proteins or confinement lead to macroscale emergent features of a full chromosome, we study megabasepair long DNA molecules in vitro. We strip, purify and reconstitute a bacterial chromosome in a microfabricated chamber or liposome, and add purified components such as SMCs or nucleoid-associated proteins. In essence, we aim to construct a full-scale in vitro model system of a chromosome.

# Rheological, structural, and physicochemical properties of heat- and cold-induced emulsion gels using myofibrillar protein or gelatin

Mi-Jung Choi <sup>a,\*</sup>

<sup>a</sup>*Department of Food Science and Biotechnology of Animal Resources, Konkuk University, Seoul, Korea*

\*Corresponding Author's E-mail: choimj@konkuk.ac.kr

---

## Abstract

The main properties of gels are particle size, shape, and structure; mechanical characteristics such as rheology, texture, and mouthfeel; and the release mechanism. These gel properties are related to consumer perception of the final product; therefore, understanding them and related techniques is important. Therefore, the aim of this study was to investigate the influence of emulsion size, different emulsifiers, and with/without trans-cinnamaldehyde (CIN) on the physicochemical properties and functionality of emulsion gels.

Gelatin emulsion–gelatin composite gels are more suitable than lecithin emulsion–gelatin composite gels owing to the weak solubility of lecithin and its inhibitory effect on protein cross-linking. Moreover, nano-sized emulsion–gelatin composite gels are more suitable than micro-sized gels, except for lecithin, owing to their high WHC, gel strength, and  $G'$  of gelatin gel formation.

In myofibrillar protein (MP) emulsion gel as an emulsifier, partial structural unfolding protein suggests the improved interfacial activity of MP in nano-emulsions, and this is supported by the confocal imaging results where MP-nano displayed numerous smaller droplets distributed within the MP matrix. Moreover, depending on the emulsion type, the secondary structure was affected.

In addition, depending on the concentration of CIN used, the emulsion gels could improve the gel strength owing to the Schiff base reaction between MPs and CIN. TBARS and ABTS tests confirmed that CIN modulated the lipid oxidation of the emulsion gel. Moreover, the effect of the emulsion droplet size was confirmed. Micro-sized emulsion gels present better physical properties than nano-sized particles because nano-sized particle do not cross-link with the emulsion gel matrix (network) in micro-sized one due to irregular self-aggregation by the high-pressure treatment.

This suggested that CIN promoted protein cross-linking because the monophenol molecule had fewer structural obstacles. The structural properties were analyzed using Fourier-transform infrared spectroscopy. It was also confirmed that lipid oxidation was inhibited by CIN.

In short, the different properties of constructed emulsion gels provided a new way for the utilization and basic data support for the construction of gel foods.



**Short Bio: Mi-Jung Choi, Professor**

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**STRENGTHS**

Critical skills and strengths include technical expertise in Food Rheology with hands-on experience in development of encapsulation formulation using polymer for functional food delivery system as well as food processing technology related with high pressure technology for development of freezing technology and freeze-drying technology.

**EDUCATION**

2001-2006      Ph.D. *La Génie Pharmaco-technique (Pharmaco-technical Engineering)*,  
Université Claude Bernard Lyon 1, Lyon, France  
1997-1999      M.S. *Food Engineering*, Konkuk University, Seoul, Korea  
1993-1997      B.S. *Food Engineering*, Konkuk University, Seoul, Korea

**RESEARCH and PROFESSIONAL EXPERIENCES**

2020-present	Professor, Konkuk University, Korea
2014-2020	Associate Professor, Konkuk University, Korea
2012-2014	Assistant Professor, Konkuk University, Korea
2010-2011	Assistant Professor, Kyonggi University, Korea
2009-2010	Research Scientist, University of Hohenheim, Germany
2007-2009	Research Scientist, National Nanotechnology Center, Thailand
2006-2007	Post-Doctoral Fellowship, Konkuk University, Korea
2001-2006	Research Assistant, Université Claude Bernard Lyon 1, France
1997-1998	Research Assistant, Animal Resources Research Center, Korea

**Teaching**

Food Engineering - undergraduate independent research course  
Physical Chemistry - undergraduate independent research course  
Food Freezing Technology - graduate level course

**GRANTS**

Establishment of lab-scale optimal temperature conditions for supercooled storage of commercial kimchi (99,000,000 KRW), 2023-2024 by World Institute of Kimchi an Annex of Korea Food Research Institute

Development and commercialization of nutrients modified therapeutic diet products for the management of kidney and diabetes diseases (410,000,000 KRW), 2022-2026 by IPET

Analysis of scalable W/O/W double emulsion formulation containing salty taste enhancer and taste material modulator mechanism (140,000,000 KRW), 2022-2024 by OTTOGI Ham Taiho Foundation

Technical development of commercialization of dried products using local agricultural products (156,000,000 KRW), 2022-2024 by RDA

Identification of interactions related to Pickering W/O/W multiphase emulsion formulation and interfacial stabilization through plant-derived protein aggregation mechanism. Supervised project manager (729,270,000 KRW), 2022-2027 by NRF

## Nanoencapsulated herbal extract: from idea to products

Neti Waranuch<sup>a,\*</sup>

<sup>a</sup>*Cosmetics and Natural Products Research Center, Faculty of Pharmaceutical Sciences Naresuan University, Phitsanulok, 65000, Thailand<sup>b</sup>*

\*Corresponding Author's E-mail: netiw@nu.ac.th

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### Abstract

Nanoencapsulation has found widespread utility across diverse applications within the domains of health and beauty industries. Extensive experimentation has been conducted to explore a myriad of encapsulated materials and methodologies, aimed at safeguarding natural functional ingredients against deleterious effects arising from hostile processing conditions and adverse storage environments. Nevertheless, the effective incorporation of nanoencapsulation into suspension and semi-solid dosage forms remains a formidable challenge. Furthermore, the scalability of production processes and the development of efficient harvesting techniques pose persistent limitations to industrial-scale implementation. This discourse endeavors to elucidate the advantages and limitations associated with select nanoencapsulation techniques for the advancement of herbal product development. Additionally, strategies for enhancing product shelf-life will be addressed, alongside an examination of pertinent clinical studies and their consequential findings.

*Keywords: Nanoencapsulation, functional ingredients, herbal products, formulation technique, clinical studies*

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Dr. Neti Waranuch is an Associate Professor in the Faculty of Pharmaceutical Sciences at Naresuan University. He attained his Ph.D. in Pharmaceutics at the University of Michigan and later did his post-doctoral training in 1998. He was also invited as a visiting researcher at the same university. Dr. Waranuch has served in numerous medical associations and board councils. He is often invited as a visiting researcher to countries like Japan and USA. Over the years, he has published more than 80 publications and has even acquired more than 30 intellectual property rights. Dr. Waranuch's Research interests lie in the area of topical drug delivery and cosmeceutical formulations. The nanoencapsulation for natural functional ingredients is also included.

# Nanotechnology Advancements in Veterinary Science: Enhancing Healthcare and Performance Across Animal Industries.

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## Abstract

In recent years, the integration of nanotechnology into the domain of veterinary medicine has generated substantial interest, offering innovative solutions to augment the efficacy and precision of therapeutic interventions. Our research endeavors have culminated in the development of a diverse array of nanocarriers, meticulously tailored to facilitate the targeted delivery of active pharmaceutical ingredients, bioactive compounds, and biopharmaceuticals, thereby addressing critical exigencies spanning aquaculture, companion animals, livestock, and poultry. Within the sphere of aquaculture, our scientific pursuit has yielded a comprehensive suite of nanovaccines, purposefully designed for both oral and immersion administration, presenting a pragmatic and efficacious alternative to conventional injection-based vaccination protocols. Expanding upon these milestones, our research has delved into the realm of herbal-based nanoparticles, harnessed as potent antimicrobial agents within the poultry industry, manifesting commendable advancements in growth performance enhancement and the mitigation of Salmonella-related challenges. Furthermore, our commitment to advancing the frontiers of veterinary science is evidenced by the innovative engineering of organic nanoparticles encapsulating modified lauric acid, which find application as formidable antimicrobial agents across various pet products. This signifies our unwavering dedication to diversifying our contributions within the veterinary landscape. Continuing to broaden the spectrum of our innovations, we have embarked upon pioneering the development of functional ingredients derived from curcumin and sesamin extract, adroitly encapsulated within nanoparticles. These avant-garde ingredients have been seamlessly integrated into premium pet foods, enriching their nutritional profiles and bestowing heightened health benefits upon our cherished animal companions. In summation, our research endeavors and accomplishments underscore the pivotal role of nanotechnology in elevating the standards of veterinary science, ensuring the well-being and performance optimization of animals across a multitude of sectors.

*Keywords: Nanoencapsulation, Veterinary Care, Vaccines, Antimicrobials, Pet Nutrition*

# Short Bio: TEERAPONG YATA, BSc, MSc, PhD

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## Education:

Degrees	Schools / University	Faculty	Major Subject	Period (Year to Year)
Doctor of Philosophy (Ph.D.)	Imperial College London, UNITED KINGDOM	Department of Medicine, Faculty of Medicine	Clinical Medicine Research	2010 – 2014
Master of Science (MSc)	Imperial College London, UNITED KINGDOM	Department of Medicine, Faculty of Medicine	Molecular Medicine	2009 – 2010
Bachelor of Science (BSc)	Chiang Mai University, THAILAND	Department of Biology, Faculty of Science	Biology	2004– 2007

## Competency:

Dr. Teerapong Yata has been an outstanding researcher in the academic field and well-accepted among the entrepreneurs in the innovative veterinary medicine industry. He received numerous awards from International Innovation competitions. In addition, he has invented several inventions and filed those innovations for patents and petty patents. His publications, which were published in remarkable international journals, mainly focus on the development of high-efficiency delivery systems using nanotechnology to deliver drugs, vaccines, biomolecules, and other bioactive compounds from herbs to be used in innovative products for disease treatment and prevention in both humans and animals.

His diligence in the development of “**Nanoparticle’s carrier for the accurate drug delivery to the body**” was recognized by the Foundation for the Promotion of Science and Technology under the Patronage of H.M. the King as he received the **Thai Young Scientist 2019** trophy from Princess Maha Chakri Sirindhorn. Moreover, he also received UK Alumni Entrepreneurship Award 2020 from British Council Thailand and British Embassy Bangkok, Thailand. This award is given to the UK alumni who initiate new innovative ideas or promising business approaches and opportunities to excel steadily. His most recent accomplishment was to be honored as a team of **outstanding young technologists 2020** with the innovation “**Pathogen-like Immersion Nano-vaccines for Fish**” from the Promotion of Science and Technology under the Patronage of H.M. the King and won the trophy from Princess Maha Chakri Sirindhorn.

## Research Expertise

The development of biomimetics, nature-inspired carriers and the application of state-of-the-art nanobiotechnology with a focus on developing innovative therapies to tackle a wide variety of diseases in both humans and animals.

## Publications

1. Tattiyapong, P., Kitiyodom, S., Yata, T., Jantharadej, K., Adamek, M., & Surachetpong, W. (2022). Chitosan nanoparticle immersion vaccine offers protection against tilapia lake virus in laboratory and field studies. *Fish & Shellfish Immunology*.
2. Thangsunan, P., Kitiyodom, S., Srisapoome, P., Pirarat, N., Yata, T., Thangsunan, P., Boonrunsiman, S., Bunnay, A., & Rodkhum, C. (2022). Novel development of cationic surfactant-based mucoadhesive nanovaccine for direct immersion vaccination against *Francisella noatunensis* subsp. *orientalis* in red tilapia (*Oreochromis* sp.). *Fish & Shellfish Immunology*, 127, 1051-1060.



## Green extraction development and biological activities of flavonoids compound in *Houttuynia cordata* Thunb. Extract for functional ingredient indicating its potential as a health product

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### Abstract

*Houttuynia cordata* Thunb. (Plu Kao) is a medicinal plant has been utilized in Thai traditional medicine and as a ingredient in health care product. This research aims to optimize the extraction factors that yield a high concentration of flavonoids. The resulting extract obtained four essential substances, including rutin, quercetin-3-D-galactoside, Quercetin-3-glucoside, and Quercetin. The biological activities assay revealed that Plu Kao extract exhibited *in vitro* antioxidant activity assessed through DPPH assay, ABTS assay, with IC<sub>50</sub> values of 11.96±0.31 and 19.11±0.39 µg/ml, respectively. The *in-situ* antioxidant activity was evaluated using DHF cell culture induced with H<sub>2</sub>O<sub>2</sub>, and statistically significant were obtained. Additionally, the extract demonstrated the capability to inhibit elastase and collagenase activities with IC<sub>50</sub> values of 89.20 ± 1.80 and 633.14 ± 34.26 µg/ml, respectively. Furthermore, the extract exhibited anti-coronavirus activity via the PLPro enzyme inhibition model with an *in vitro*, IC<sub>50</sub> of 405.5 µg/ml. The permeability study conducted on Caco-2 cells suggest that Plu Kao extract can be absorbed through the intestinal mucosa, Stability test of Plu Kao extract indicating favorable chemical stability, with active substances showing changes of no more than 10% of the initial volume. The extract exhibited melting behavior at 50°C. To enhance its physical stability, it is recommended to include maltodextrin during further extraction processes or develop encapsulated forms of Plu Kao extract to improve stability, solubility, and permeability. Moreover, a comprehensive analysis confirmed the absence of contaminated microorganisms and heavy metals, certifying the suitability of the raw materials for the development of functional ingredients indicating its potential as a health product.

**Keywords:** *Houttuynia cordata* Thunb., Green extraction, biological activity, functional ingredient, health care product

**Short Bio:**

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**EDUCATION**

- 2009-2011: Postdoctoral fellowship at Kobe Pharmaceutical University, Kobe, Japan on a project entitled “Regulation of immune disease by monoclonal antibodies to pathogenic antigens” (Nov. 2009- Oct. 2011)
- 2008: The Degree of Doctor of Philosophy in Biomedical Chemistry, Department of Biochemistry, Faculty of Pharmaceutical Science, Chulalongkorn University, Bangkok, Thailand.  
Dissertations Title: Cloning and expression of amorpha-4,11-diene synthase gene in *Artemisia annua*
- 2003: The Master of Science in Biomedical Chemistry, Department of Biochemistry, Faculty of Pharmaceutical Science, Chulalongkorn University, Bangkok, Thailand  
Thesis Title: Potential of Artemisinin Production in *Artemisia annua* Mutants
- 2000: The Bachelor of Science in Biochemistry, Department of Biochemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand
- 1998: The Diploma of Analytical Chemistry Training, Department of Science service, Ministry of Science, Technology and Environment, Bangkok, Thailand (Affiliated Institute of Chulalongkorn University)

**AWARD**

- 2022: Gold Prize, SEOUL INTERNATIONAL INVENTION FAIR 2022, “REISHURAL: ESSENTIAL NATURAL FACIAL SERUM, From Encapsulation technology to cosmetic Innovation” Seoul, SOUTH KOREA
- 2022: Silver Medal, “SPECIAL EDITION 2022 - INVENTION GENEVA EVALUATION DAYS”, “REISHURAL: NATURAL FACIAL SERUM, From Encapsulation technology to cosmetic Innovation” Geneva, SWITZERLAND
- 2010: Inventor Award 2010 on “Portable Thin Layer Chromatography Kit for Artemisinin Analysis” from National Research Council of Thailand 2010: Portable Thin-Layer Chromatography Kit for Artemisinin Analysis. Department of Intellectual Property, THAILAND.

**PUBLICATIONS**

- 2021: Nalinrat Petpiroon, Apiwan Rosena, Wittaya Pimtong, Sawanya Charoenlappanit, **Thongchai Koobkokkruad**, Sittiruk Roytrakul, Sasitorn Aueviriyavit. Protective effects of Thai silk sericins and their related mechanisms on UVA-induced phototoxicity and melanogenesis: Investigation in primary melanocyte cells using a proteomic approach. *International J. Biol. Macromol.* 201: 75-84.
- 2019: **Thongchai Koobkokkruad**, Praderm Wanichananan, Chalermopol Kirdmanee and Wanchai De-Eknamkul. Gamma Irradiation Causes Variation and Stability of Artemisinin Content in *Artemisia annua* Plants. Use of Gamma Radiation Techniques in Peaceful Applications, Chapter 14 Edited by Basim Almayahi Licensee IntechOpen.
- 2019: Supakanya Kumkarnjana, Rutt Suttisri, Ubonthip Nimmannit, Apirada Suontphunt, Mattaka Khongkow, **Thongchai Koobkokkruad**, Nontima Vardhanabhuti. Fvonoids kaempferide and 4,2'-dihydroxy-4',5',6'-trimethoxychalcone inhibit mitotic clonal expansion and induce apoptosis during the early phase of adipogenesis in 3T3-L1 cells. <https://doi.org/10.1016/j.joim.2019.04.004>
- 2018: Worapan Sitthithaworn, Mattaka Khongkaw, Chutima Wiranidchapong, and **Thongchai Koobkokkruad**. Mucilage powder from *Litsea glutinosa* leaves stimulates the growth of cultured human hair follicles. *Songklanakarin J. Sci. Technol.* 40 (5), 1076-1080

## "Enhancing Anti-Inflammatory Potential: Ginger-Gold Liposomes with Iontophoresis for Skin Effect"

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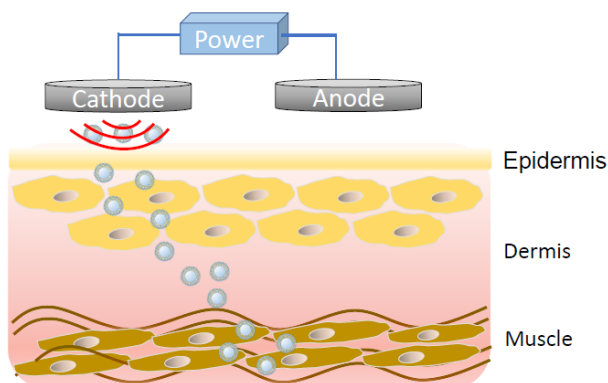
### Abstract

Ginger root extract and gold nanoparticles are renowned for their anti-inflammatory properties. However, the limited solubility and stability of ginger extract hinder its practical applications. This study addresses this challenge by encapsulating ginger root extract within liposomes, thereby enhancing its stability. Furthermore, the research combines ginger root extract with gold nanoparticles within these liposomes, offering a dual anti-inflammatory action. Results unequivocally demonstrate that these ginger-gold liposomes exhibit robust inhibition of nitric oxide and TNF-alpha, both key inflammatory mediators.

To expand the utility of this innovation, a ginger-gold liposome emulgel for topical application on the skin was formulated. Remarkably, this emulgel exhibited stability throughout six heating-cooling cycles. To maximize the skin penetration of these liposomes, iontophoresis was employed as a facilitating technique. Fluorescent imaging corroborated significantly higher cellular uptake and deeper skin penetration when iontophoresis was applied to activate the liposomes.

This research presents a promising strategy for harnessing the potent anti-inflammatory properties of ginger and gold nanoparticles through liposomal encapsulation, culminating in a stable emulgel with enhanced skin penetration capabilities, holding potential for therapeutic applications in inflammatory skin conditions.

*Keywords: green synthesis, stimulus-responsive materials, ginger, natural inspire*



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**Education**

Doctor of Philosophy in Pharmaceutical Sciences, University of Michigan, 2017.  
Master of Science in Pharmaceutical Sciences, University of Michigan, 2014.  
Bachelor's degree of Pharmacy and Pharmaceutical Sciences (Major Pharmaceutics), First Class Honours, Chulalongkorn University, Bangkok, Thailand, 2007

**Research Interests**

Nanoparticles for drug carriers, imaging, photothermal therapy, ionizing radiation, cancer vaccines, immunotherapy, and bone regeneration

**Peer Reviewed Publications**

1. Sansanaphongpricha, K.; Sonthithai, P.; Kaewkong, P.; Thavornnyutikarn, B.; Bamrungsap, S.; Kosorn, W.; Thinbanmai, T.; Saengkrit, N. Hyaluronic Acid-Coated Gold Nanorods Enhancing BMP-2 Peptide Delivery for Chondrogenesis. *Nanotechnology* 2020, 31.
2. Sansanaphongpricha, K.; DeSantis, M. C.; Chen, H.; Cheng, W.; Sun, K.; Wen, B.; Sun, D. Multibuilding Block Janus Synthesized by Seed-Mediated Self-Assembly for Enhanced Photothermal Effects and Colored Brownian Motion in an Optical Trap. *Small* 2016, 1602569, 1–11.
3. Tan, Y. S\*; Sansanaphongpricha, K\*; Xie, Y.; Donnelly, C. R.; Luo, X.; Heath, B. R.; Zhao, X.; Bellile, E. L.; Hu, H.; Chen, H.; et al. Mitigating SOX2-Potentiated Immune Escape of Head and Neck Squamous Cell Carcinoma with a STING-Inducing Nanosatellite Vaccine. *Clin. Cancer Res.* 2018. \*Equally contributed
4. Luan, X\*; Sansanaphongpricha, K\*; Myers, I.; Chen, H.; Yuan, H.; Sun, D. Engineering Exosomes as Refined Biological Nanoplatfroms for Drug Delivery. *Acta Pharmacol. Sin.* 2017, 1–10. \*Equally Contributed 2
5. Laksee, S.; Sansanaphongpricha, K.; Puthong, S.; Sangphech, N.; Palaga, T.; Muangsin, N. New Organic/Inorganic Nanohybrids of Targeted Pullulan Derivative/Gold Nanoparticles for Effective Drug Delivery Systems. *Int. J. Biol. Macromol.* 2020, 162, 561–577.
6. Sansanaphongpricha, K., Dana, P., Yata, T., & Saengkrit, N. (2021). Cancer nanomedicine. In U. R. R. Woei Jye Lau, Kajornsak Faungnawakij, Kuakoon Piyachomkwan (Ed.), *Handbook of Nanotechnology Applications* (pp. 537–566). Elsevier. <https://doi.org/10.1016/B978-0-12-821506-7.00021-1>
7. Sangjan, A., Boonsith, S., Sansanaphongpricha, K\*\*, Thinbanmai, T., Ratchahat, S., Laosiripojana, N., Wu, K. C.-W., Shin, H. S., & Sakdaronnarong, C\*\*. (2022). Facile preparation of aqueous-soluble fluorescent polyethylene glycol functionalized carbon dots from palm waste by one-pot hydrothermal carbonization for colon cancer nanotheranostics. *Scientific Reports*, 12(1), 10550. <https://doi.org/10.1038/s41598-022-14704-x> \*\* Co-corresponding authors
8. Hongsa, N., Thinbanmai, T., Luesakul, U., Sansanaphongpricha, K\*\*, & Muangsin, N\*\*. (2021). A novel modified chitosan/collagen coated-gold nanoparticles for 5-fluorouracil delivery: Synthesis, characterization, in vitro drug release studies, anti-inflammatory activity and in vitro cytotoxicity assay. *Carbohydrate Polymers*, 277(November 2021), 118858. <https://doi.org/10.1016/j.carbpol.2021.118858> \*\* Co-corresponding authors
9. Suksiri, P., Sansanaphongpricha, K., & Muangsin, N. (2023). Development of positively-charged cycloamylose, CAQ as efficient nanodelivery system for siRNA. *Biochemical Engineering Journal*, 191(December 2022), 108767. <https://doi.org/10.1016/j.bej.2022.108767>
10. Chen, H.; Luan, X.; Paholak, H. J.; Burnett, J. P.; Stevers, N. O.; Sansanaphongpricha, K.; He, M.; Chang, A. E.; Li, Q.; Sun, D. Depleting Tumor-Associated Tregs via Nanoparticle-Mediated Hyperthermia to Enhance Anti-CTLA-4 Immunotherapy. *Nanomedicine (Lond)*. 2020, 15 (1), 77–92.

## Green synthesis of silver nanoparticles from *Nigella sativa* seeds extract: A promising natural approach for enhanced wound healing via PDGF and VEGF signalling pathways activation

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### Abstract

Silver nanoparticles (AgNPs) show promise for wound healing due to their antimicrobial and pro-healing properties. However, their conventional synthesis methods often involve toxic chemicals, raising environmental concerns. This study introduces a green synthesis method utilizing *Nigella sativa* (N. sativa) seed extract (NSSE) as a reducing and stabilizing agent for AgNPs production. Various analytical techniques, including UV-Visible spectroscopy, FTIR, XRD, SEM, and DLS, confirmed the size, shape, stability, and composition of AgNPs-NSSE. In vitro studies demonstrated enhanced proliferation and migration of HaCat cells treated with AgNPs-NSSE compared to controls. Additionally, increased expression of platelet-derived growth factor (PDGF) and vascular endothelial growth factor (VEGF), crucial in wound healing, was observed in AgNPs-NSSE. These findings suggest AgNPs-NSSE's potential as a natural wound healing agent, possibly due to activation of PDGF and VEGF signaling pathways. Future research should delve into underlying molecular mechanisms and assess the long-term safety and efficacy of green-synthesized AgNPs.

**Keywords:** *Nigella sativa* seeds extract, Green synthesis, Silver nanoparticles, Wound healing, PDGF, VEGF.



# Imitated Melanin Particles: Hollow Polydopamine Synthesis and Its Application in Sunscreen Product

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## Abstract

Sunscreen products are important in blocking ultraviolet (UV) radiation from the sun, which causes sunburn, freckles, and skin cancer. The safety of active ingredients in sunscreen is a major factor to be aware of when using them in products and humans. This research aims to synthesize hollow polydopamine (h-PDA) particles that mimic melanin structure in human skin. It is thought to be the most compatible when applying it to the skin. The particles were successfully synthesized using the hard-template method under weak alkaline condition in the presence of tris-(hydroxymethyl)aminomethane (Tris) as a catalyst. Dopamine hydrochloride (DA) monomer was gradually converted to polydopamine particles (PDA) by spontaneous polymerization on a polystyrene (PS) core template. Effect of size of the core template and weight ratio of PS to DA monomer on morphology and UV absorption ability of the h-PDA were investigated. Results revealed that, at a similar shell thickness, the h-PDA particle with a larger void diameter (~ 450 nm) exhibited higher UV absorption than that of a smaller void. Characterization of chemical structure of the h-PDA particles suggested that the synthesized particles majority consisted of a mixture of 5,6-dihydroxyindole (DHI) and indole-5,6-quinone (IQ) precursors covalently linked together and dominated in the form of the DHI group compared to IQ group. Furthermore, the particles were remarkably stable after storage under high temperature 50 degree Celsius for 3 months. After using h-PDA particles as an active ingredient in sunscreen product by merging with pristine base cream, the formulation contained the h-PDA having a larger void diameter displayed the highest sun protection factor (SPF) up to 234.7% compared to the pristine base cream. In addition, the h-PDA particles exhibited superior biocompatibility with no mutagenicity and were non-irritant tested according to OECD TG 471 and OECD 439, respectively.

*Keywords: polydopamine, hollow structure, sunscreen particles, biocompatible*

## Simple Method to Increase the Liposomes Stability and Encapsulation Efficiency

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### Abstract

Liposomes are commonly used as active compounds delivery vehicles for both hydrophilic and hydrophobic compounds. The nanoparticles have many advantages, such as stabilizing and decreasing the potential side effects of the active compounds, making the structure popular in medical and cosmetic/cosmeceutical applications. Liposomes' structure and components also resemble that of biological cell membrane, making them biocompatible. However, the nanoparticles still have problems with the low encapsulation efficiency and structure's stability. Here, a simple method to increase the encapsulation efficiency of the liposomes was investigated. That was, the inclusion of anionic lipid into the neutral liposomes structure and the addition of polymer to the core part to make it more viscous. Results showed that the presence of both factors has the tendency to significantly impact the liposomes' characteristics and the percent encapsulation efficiency. Release mechanisms of different liposome formulations were also studied to investigate the effects of two factors included into the formulations on their release fashion. In conclusion, this work presents a simple method that can be further applied in the development of high stability liposomes.

*Keywords: Encapsulation Efficiency, Liposome, Stability*

## Panitumumab modified 5,7-dimethoxyflavone loaded-liposome improves targeting and therapeutic efficacy on prostate cancer cells

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### Abstract

Prostate cancer is the second most common male malignancy cancer. Chemotherapy is widely used for prostate cancer treatment. However, its therapeutic effectiveness is limited owing to cancer chemoresistance and side effects on non-cancer cells. Here, the black ginger (*Kaempferia parviflora*)'s active ingredient (5,7-dimethoxyflavone (DMF)) was used as anti-cancer compound and panitumumab was conjugated to liposome. Panitumumab was selected since it could precisely target epidermal growth factor (EGFR) which overexpress in prostate cancer cells. The present study aims i) to develop DMF loaded-liposome (LD) and panitumumab modified LD (Pan-LD), ii) to evaluate its cellular uptake efficacy on prostate cancer cell (PC3) and iii) to study the anti-cancer effect of LD and Pan-LD on PC3. The synthesized LD and Pan-LD were in a nanosized, with a neutral charge and narrow dispersity index (<0.2). The encapsulation efficiency of LD and Pan-LD were approximate 50%. During 72 hours of an *in vitro* release study, only 40% of DMF was released from Free D, with a burst release in the first hour while 90% of DMF was slowly released from LD, with nearly 70% and 90% in 24 hours and 72 hours, respectively. Flow cytometry analysis showed significant higher cellular uptake of coumarin-6-labeled panitumumab modified liposome (Pan-LC6), compared to coumarin-6-labeled nonmodified liposome (LC6) at 1 hour ( $p < 0.01$ ). MTT analysis demonstrated that Free D, LD, and Pan-LD inhibit the proliferation of PC3 cells in dose-dependent manner. Interestingly, the percent cellular viability of PC3 after treatment with Pan-LD at the dose of 6.25 and 12.5  $\mu\text{g/ml}$  ( $56.02 \pm 2.10$  and  $49.26 \pm 0.93$ ) were statistically significantly lower ( $p < 0.01$  and  $p < 0.05$ , respectively), compared to those treatment with LD at the similar doses ( $70.59 \pm 5.69$  and  $59.59 \pm 4.65$ ). In conclusion, Pan-LD enhanced the anti-cancer effects of LD on PC3 cells, possibly due to an EGFR-targeting capacity.

**Keywords:** EGFR, epidermal growth factor, *Kaempferia parviflora*, *Krachaidum*

## Resveratrol-loaded liposomes for Targeting and Reprogramming Cancer-Associated Fibroblasts in Prostate Cancer

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### Abstract

The progression of tumor requires the support from their tumor microenvironment (TME). Cancer-associated fibroblasts (CAFs), the most abundant stromal cells infiltrating in TME, play vital roles in secreting of growth factors, cytokines, and extracellular matrix to enhance tumor development and aggressiveness. Therefore, targeting and reprogramming of CAFs have become a promising strategy to improve cancer treatment outcome. Resveratrol (Res) has been widely explored its application in cancer therapy, and ability in interrupting the crosstalk between CAFs and cancer cells. However, limitation of Res is poor water solubility resulting in low bioavailability in clinical used. The present study aimed to enhance bioavailability, specificity, and prolonging the activity of Res by using targeted nano-drug delivery system in prostate cancer cells. Res was encapsulated into liposomes. The liposomes were surface decorated with anti-human fibroblast activation protein- $\alpha$  monoclonal antibody (anti-FAP) to target CAFs yielding Lip/Res/anti-FAPs. The obtained Lip/Res/anti-FAPs provided the diameter length of  $185.40 \pm 5.70$  nm with the zeta potential and poly dispersity index values of  $1.16 \pm 0.20$  mV and  $0.32 \pm 0.02$ , respectively. The encapsulation efficiency of Res was  $99.7 \pm 0.02$  %. The *in vitro* release experiment revealed that the liposomes can prolong the release of Res to 72 h, while free Res completely released within 6 h. The *in vitro* cytotoxicity of Lip/Res/anti-FAPs against fibroblasts was investigated. In addition, Lip/Res/anti-FAPs demonstrated their ability in suppressing the activity of prostate cancer-activated fibroblasts via the reduction of  $\alpha$ -smooth muscle actin expression and matrix metalloproteinase-2 secretion. Taken together, Lip/Res/anti-FAPs exhibited a promising outcome as a drug delivery system to target CAFs in TME due to their proper characteristics, controlled release profile, and the ability in deactivating of activated fibroblast. This study proposes an alternative approach of cancer treatment and could be applied as a combination treatment with chemotherapeutics.

**Keywords:** resveratrol, targeting liposome, fibroblast activation protein, cancer-associated fibroblast, prostate cancer

# Synthesis of Lipid Nanoparticles-Based RNA Delivery Using Microfluidic Technology

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## Abstract

A challenge to mRNA-based vaccine is to deliver the genetic material into cell in which the mRNA is not damaged by human immune system. To overcome this issue, lipid-based nanoparticles are the most effective tool for the delivery of mRNA. Recently, microfluidic technology is of great interest to produce lipid nanoparticles (LNPs) since LNPs with precisely defined properties can be generated using microfluidics. In this work, we present the design and fabrication of microfluidic devices to encapsulate the state of genetic material inside lipid nanoparticles based on X-ray lithography technique available at BL6: DXL, SLRI. Typically, liquids in a microfluidic system have a laminar flow. In order to generate mixing in this situation, the design of microfluidic structure in this work, consisting of a chain of elements based on staggered herringbone, was placed in the channel to create a more efficient turbulent flow inside the microchannel and thus a mixing process was achieved. Using this designed structure, lipid nanoparticles encapsulating ssDNA with a diameter less than 100 nanometer have been produced with the flow rate ratio (FRR) between the lipid solution and the genetic material solution of 1:6. Furthermore, a more detailed description of the lipid nanoparticles-based ssDNA has been characterized using synchrotron-based X-ray scattering at BL1.3: SAXS. It was confirmed that the structure was organized in a Uni-Lamellar Vehicle (ULV) with a  $d$ -spacing of 3.4 nm. Moreover, it provided an entrapment ratio (ER) of about 94% protecting DNA from degradation when exposed to the DNase I enzyme for a duration of 2-16 hours. In addition, toxicity to THP-1 at concentrations ranging from 0 to 400 ppm and HEK293T at concentrations from 0 to 2000 ppm were not detected demonstrating the capabilities of in-house developed quantitative vaccine production devices in the future.

*Keywords: Lipid nanoparticles-based RNA, Nanoencapsulation, Microfluidics, X-ray lithography, X-ray scattering*



# Characterization and In Vitro Digestibility of Colostrum Whey based Nanoparticles through the Structural Modification of Proteins with Ethanol

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## Abstract

Bovine colostrum contains a high number of bioactive proteins while thermal processing reduces the functionality of these proteins and gastric conditions also reduce the bioactivity of these proteins. The functionality of whey can be enhanced by modifying the structure with amphiphilic solvents such as ethanol and fabricating NPs can impart extra stability to sensitive proteins in the gastric phase. In this study, the structure of caseinate and colostrum whey was modified using ethanol to fabricate the nanoparticle (NPs) with improved functionality and bioaccessibility of Immunoglobulins. The effect of pH (4-7), whey (0.25-1.0%, w/v), and caseinate (0.5-2.0%, w/v) concentrations was also evaluated to fabricate stable NPs. The stable NPs were prepared at pH 6.5 using caseinate (1.50%, w/v) and whey (0.75%, w/v) in an aqueous medium with a mean particle diameter of <200 nm. The differential scanning calorimetry showed that the thermal stability of NPs was slightly higher (116.50 °C) compared to native proteins. The FTIR assay confirmed that the secondary structures ( $\alpha$ -helix  $\sim 1650\text{ cm}^{-1}$ , amide II  $\sim 1530\text{ cm}^{-1}$ , and amide I  $1250\text{-}910\text{ cm}^{-1}$ ) of proteins remained unaltered. The NPs in an aqueous medium showed good stability for 5 days at 25 °C. The functionality and bioaccessibility of Igs were improved for NPs as compared to whey and caseinate. These colostrum whey-based NPs can be used as dietary supplements to deliver bioactive proteins with numerous health advantages.

**Keywords:** Caseinate, Colostrum, Functionality, Nanoparticles, Whey

## Characterization and Stability Evaluation of Extracted *Mitragyna speciosa* (Kratom) Nanoemulsion

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### Abstract

In Thailand, *Mitragyna speciosa* (Kratom) leaves have been used for enhancing work productivity and especially pain relief, due to the opioid agonistic activities of mitragynine, an indole alkaloid only found in kratom leaves. However, its applications in medicinal and pharmaceutical industries are limited due to its poor aqueous solubility and low stability under light and heat. Therefore, Nanoencapsulation technology is utilized to solve these problems by using oil in water (o/w) nanoemulsion system. In this work, extracted kratom nanoemulsions were formulated using low energy method at 60-70°C. The optimized nanoemulsions consist in form of percent by weight; 2% oil phase, 10-20% surfactant; tween 80, 1% glycerin, and water phase. Prepared nanoemulsions were characterized in terms of appearance, particle size, zeta potential value, polydispersity index (PI), pH value, and their stability. The results showed decreasing of particle size and PI when the concentrations of tween 80 increased. The particle sizes were about 15-110 nm. Zeta potential values were lower than -30 mV indicating good stability. In 90 days, larger size of particle in nanoemulsions was observed in longer time storage, high temperature (50°C), and basic environment. However, zeta potential values of nanoemulsions were slightly changed under these conditions.

*Keywords: Mitragynine, Kratom, Nanoemulsion*

# Effect of Trans-Cinnamaldehyde on the Textural Properties of Myofibrillar Protein Gels Filled Micro- and Nano-Sized Emulsions

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## Abstract

Trans-cinnamaldehyde (CIN) has antioxidant and antimicrobial properties and reduces total cholesterol and glucose levels in the blood. However, CIN in the food system is limited due to poor water solubility. Emulsion gels are a composite structure composed of oil droplets within a gel matrix, preventing flocculation and coalescence of oil droplets and acting as control release systems. Therefore, in this study, we investigated the influence of trans-cinnamaldehyde (CIN) and emulsion size on the physicochemical properties and functionality of emulsion gels. Myofibrillar protein or lecithin emulsions were fabricated with different ratios of canola oil and CIN and different emulsion droplet sizes. The emulsion gels showed a significant dependence on CIN concentration in terms of gel strength and rheological properties because of the improved interaction between proteins and aldehydes through the Schiff base reaction. In addition, the physical properties of the micro-sized emulsion gels were better than those of the nano-sized gels. There was no significant difference in the water-holding capacity. According to the scanning electron and confocal microscopy images, the CIN emulsion gels formed a denser microstructure and had a higher homogeneity with higher CIN concentrations. This suggested that CIN promoted protein cross-linking because the monophenol molecule had fewer structural obstacles. The structural properties were analyzed using Fourier-transform infrared spectroscopy. It was also confirmed that lipid oxidation was inhibited by CIN. The information obtained in this study could be used to develop protein-based products with novel functional properties for use in meat products and other applications.

*Keywords: Micro-sized emulsion, nano-sized emulsion, myofibrillar protein, emulsion gel, trans-cinnamaldehyde*

# High Internal Phase Emulsions Stabilized Solely by Mung Bean Protein Isolate at Various pHs: Effect of Heat Treatment and Ultrasonication

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## Abstract

This work aimed to investigate the impact of pretreatments on the structural properties of mung bean protein isolates (MBPIs) and to compare their emulsifying properties when they applied to high internal phase emulsions (HIPEs). MBPIs were heat-alone treated or sequentially heat and ultrasound treated at various pHs (pH 2, pH 7 and 10) and 0.7 of the oil fraction was used for manufacturing HIPEs. The surface hydrophobicity increased approximately 2-folds ( $p < 0.05$ ) when samples were heated (90°C, 2 h) at all pHs, whereas ultrasonication after heated MBPIs was not significantly different from that of MBPI heat-alone treated ( $p > 0.05$ ). FT-IR spectroscopy revealed that both heat treatment and sequential ultrasonication induced changes in secondary structure, with an increase in  $\beta$ -sheet and a decrease in  $\alpha$ -helix indicating the exposure of hydrophobic groups and the disruption of hydrogen bonds. Through solubility and turbidity results, the protein aggregates tend to exist as soluble aggregates after heating and ultrasonication, except heat treated MBPI at pH 7. The particle size and PDI values of MBPIs decreased after heat and ultrasonication, regardless of pH, due to thermal energy and cavitation effects, respectively. Consequently, ultrasonication disrupts intermolecular bond between soluble or insoluble aggregates and decrease aggregates size, with not decreasing hydrophobicity ( $p > 0.05$ ). Furthermore, the characteristics of the HIPEs stabilized by those MBPIs were investigated and the particle size,  $\xi$ -potential and rheological properties of HIPEs were analyzed. At all pHs, heating and ultrasonication treatments were involved in reducing the size of HIPEs ( $p < 0.05$ ) due to increased surface hydrophobicity, compared to the HIPEs emulsified with untreated MBPIs. The HIPEs emulsified with pH 10 MBPIs showed low viscoelasticity, correlating with fast adsorption of small size MBPIs at oil/water interface, forming small emulsion droplets. This work may provide insight into the interfacial and emulsifying properties of heated and ultrasonicated MBPIs at various pHs.

*Keywords: Mung bean protein isolates, heat treatment, ultrasonication, high internal phase emulsion*

# Synthesis of Cellulose Paper from Sugar Cane Leaves Filled with Zinc Oxide Nanoflakes for Triboelectric Nanogenerator Application to Harvest Mechanical Energy

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## Abstract

The triboelectric nanogenerator (TENG) is a new emerging energy technology that converts mechanical energy in the environment into electricity, based on contact electrification and electrostatic induction. In this research, cellulose paper is synthesized from sugarcane leaves to fabricate a triboelectric nanogenerator (TENG). Cellulose paper is modified by zinc oxide (ZnO) nanoflakes, which are prepared by the precipitation of zinc acetate dihydrate ( $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ ) and sodium hydroxide (NaOH). ZnO nanoflakes are grown on cellulose fibers with different sizes and shapes with presence of ethylenediamine ( $\text{NH}_2(\text{CH}_2)_2\text{NH}_2$ ; EDA). The influence of ZnO nanoflakes prepared at different synthesis conditions on the electrical output of TENG is investigated. It is found that the concentration of sodium hydroxide significantly affects the growth volume of ZnO nanoflakes. Cellulose paper modified with ZnO shows improved TENG performance, which can be used as a power supply for portable electronic devices and motion sensors. This research not only presents a strategy to increase the performance of TENG, but also proposes the use of sugarcane leaves which are an agricultural waste material to develop a clean and sustainable power source.

**Keywords:** Cellulose paper, Triboelectric nanogenerator, ZnO nanoflakes, Sugarcane leaves

# Computational Studies of Nanomaterials using DCDFTBMD Program

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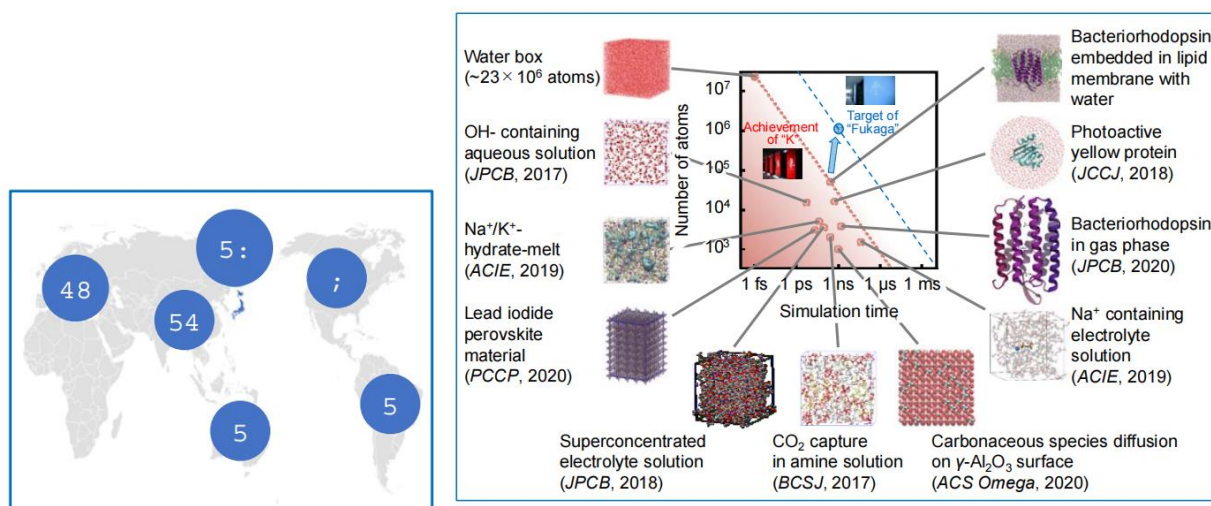
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## Abstract

Our research group has developed the massively parallel DCDFTBMD program [1], which combines the divide-and-conquer type density-functional tight-binding (DCDFTB) method [2] with the molecular dynamics (MD) simulation technique in the last decade. The DCDFTBMD program can treat the electronic structures of huge systems such as 100 million atoms [3]. Since the release on November 2018, 75 research groups in 22 countries has registered to use the DCDFTBMD program. We also applied the DCDFTBMD program to nano materials to examine the dynamical properties not only in the ground state but also in the excited states. In the presentation, I will explain the performance of the DCDFTBMD program and then introduced several applications such as high proton diffusivity in organo-metallic nanotube [5] and charge-transfer dynamics in organic photo-voltaic interface [6].



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- [4] <http://www.chem.waseda.ac.jp/dcdftbmd/>
- [5] K. Otake, et al., Nature Comm., 11, 843 (2020).
- [6] H. Uratani, H. Nakai, J. Phys. Chem. Lett., 14, 2292 (2023).

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**Education:**

- 1983–1987 Department of Chemical Engineering, Faculty of Engineering,  
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Awarded the degree of Bachelor of Engineering
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- 1987–1992 Dept. of Synthetic Chemistry and Biological Chemistry,  
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- 1992–1996 Research Associate at the Dept. of Synthetic Chemistry and Biological Chemistry,  
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- 1996–1998 Assistant Professor at the Department of Chemistry,  
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- 1998–2004 Associate Professor at the Department of Chemistry,  
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- 2004–2007 Professor at the Department of Chemistry,  
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- 2007– present Professor at the Department of Chemistry and Biochemistry,  
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**Extra Research and Professional Experience:**

- 1997–1998 Visiting Lecturer at the Department of Synthetic Chemistry and Biological Chemistry,  
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- 2002–2003 Visiting Professor at the Department of Chemistry, Rice University  
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- 2006–present Trustee at the Quantum Chemistry Research Institute (QCRI)
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- 2010–2011 Visiting Professor at the Department of Theoretical and Computational Molecular Science,  
Institute for Molecular Science (IMS), National Institutes of Natural Sciences (NINS)
- 2011–2012 Visiting Professor at the Institute for Materials Chemistry and Engineering, Kyushu University
- 2011–2018 Vice Chair at the Waseda Institute for Science & Engineering (WISE), Waseda University
- 2012–2021 Visiting Professor at the Elements Strategy Initiative for Catalysts and Batteries (ESICB),  
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# Charge separation and exciton structure in graphene quantum dots and carbon nitride quantum dots

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## Abstract

Graphene quantum dots (GQDs) and Carbon nitride quantum dots (CNQDs), the latest addition to the carbon material family promise numerous novel applications in optical sensing, photo-catalysis, bio-sensing, and photovoltaics. However, understanding the photocatalytic capability of CNQDs compared to the graphene quantum dots (GQDs) have not been investigated thoroughly. In this work, through time-dependent density functional tight binding (TD-DFTB) calculations, it is revealed that due to the ground state frontier molecular orbitals (FMOs) localization, CNQDs have superior carrier charge separation, sensitive to the size of the QD. Strong localization of the FMOs and excited state charge separation was observed in the first excited state due to the relaxation of the structure. The exciton structure reveals spatial confinement to the stretched C-N bonds independent of the size of the QDs while there is no such exciton structure found for GQDs. The optical absorption and emission of CNQDs is sensitive to size and does not show strong variations in the shape of the QD. Our approach provides an explanation for the origin of the enhanced photocatalytic performance of CNQDs over graphene quantum dots (GQDs) and their characteristic exciton localization.

*Keywords: Graphene quantum dots, carbon nitride quantum dots, exciton, charge separation, confinement*

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Chair Professor, Department of Physics, City Univ. Hong Kong (1/7/2019-)  
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Professor, Department of Physics, City Univ. Hong Kong (1/7/2017-31/6/2019)  
Professor, Department of Physics and Materials Science, City Univ. Hong Kong (1/9/2010-31/6/2017)  
Associate Professor, City University of Hong Kong (1/7/2004 -31/8/2010)  
Assistant Professor, City University of Hong Kong (1/9/1998 -30/6/2004)  
Research Fellow, City University of HK (6/1997 -9/1998)  
Invited Scientist, University of Barcelona, Spain (6/1995 -6/1997)  
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**Research Background:**

Energetics, kinetics and dynamics involved in formation/growth/reaction of low-dimensional functional materials and the materials' novel properties studied using computational and experimental approaches. The theoretical and computational approaches adopted include optimization algorithms, molecular dynamics simulations and Monte Carlo methods, based on multi-level theories ranging from molecular mechanics, semiempirical theories, to first-principles theories. Recent research focus is on nanoscience, including interactions of nanomaterials with chemical, biological, and medical systems, aiming at promoting the applications of nanostructured materials in energy-related and chemical, biological, medical, and environmental areas. Developments of related theories and methodologies.

**Publication record:**

**450 SCI papers (~13500 citations and h-index=55**, as shown in

<https://www.scopus.com/authid/detail.uri?authorId=55277269000>), 7 book chapters, 2 monographs

**Section A - Five most representative publications in recent five years (\* corresponding author)**

- A1) H.R. Tian, Y.L. Zhao, M. T. Oo, F. Huang, M. Huang, W. Xiong, Y. Yu, and R.Q. Zhang\*, "Charge Transfer Doping of Carbon Nitride Films Through Noncovalent Iodination for Enhanced Photoelectrochemical Performance: Combined Experimental and Computational Insights", *Small*, 2200510 (2022).
- A2) M. Huang, H. Wang, W. Li, Y.L. Zhao\*, Rui-Qin Zhang\*, "In-situ textured carbon nitride photoanodes with enhanced photoelectrochemical activity by bandgap state modulation", *J. Mater. Chem. A* 8, 24005-24012 (2020)
- A3) W. Xiong, H. Wang, Z. Wang, F. Huang, T. Dudka, Z. Lu, Y. Zhao\*, Rui-Qin Zhang\*, "A pseudo-metal-free strategy for constructing high performance photoelectrodes", *J. Mater. Chem. A* 8, 25, 12767-12773 (2020)
- A4) Y. Guo, S. Chen, Y. Yu\*, H. Tian, Y. Zhao, J.C. Ren, C. Huang, H. Bian, M. Huang, L. An, Y. Li, R.Q. Zhang\*, "Hydrogen-Location-Sensitive Modulation of the Redox Reactivity for Oxygen-Deficient TiO<sub>2</sub>", *J. Am. Chem. Soc.* 141, 8407-8411 (2019).
- A5) Y.G. Yu, X. Yang, Y.L. Zhao, X.B. Zhang, L. An, M.Y. Huang, G. Chen, and R.Q. Zhang\*, "Engineering the Band Gap States of the Rutile TiO<sub>2</sub>(110) Surface by Modulating the Active Heteroatom", *Angew. Chem. Int. Ed.* 57, 8550–8554 (2018).

**Section B - Five representative publications beyond the recent five-year period**

- B1) J. Bian, L.F. Xi, C. Huang, K. M. Lange, R.Q. Zhang\*, M. Shalom, "Efficiency Enhancement of Carbon Nitride Photoelectrochemical Cells via Tailored Monomers Design", *Adv. Energy Mater.* 1600263 (2016).
- B2) J. Bian, Q. Li, C. Huang, J. Li, Y. Guo, M. Zaw, R.Q. Zhang\*, "Thermal Vapor Condensation of Uniform Graphitic Carbon Nitride Films with Remarkable Photocurrent Density for Photoelectrochemical Applications", *Nano Energy* 15, 353–361 (2015).
- B3) J. Bian, C. Huang, L. Wang, W. A. Daoud, R.Q. Zhang\*, "Carbon dot loading and TiO<sub>2</sub> nanorod length dependence of photoelectrochemical properties in carbon dot/TiO<sub>2</sub> nanorod array nanocomposites", *ACS Applied Materials & Interfaces* 6 (7), 4883–4890 (2014).

# Heterogeneous Catalysts Screening with the help of Quantum Chemistry and Machine Learning: A case of high-entropy alloys

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## Abstract

The screening of heterogeneous catalysts relies mostly on experimentations, e.g., surface characterizations, chemical property determinations, and reaction testing. However, screening in a large pool of catalytic materials for candidates via experimentations alone requires intensive amounts of chemicals and time being used during catalyst preparation, characterization, and reaction testing. Thus, computational techniques based on quantum chemistry, such as Density Functional Theory, have been extensively employed to speed up the pre-screening process of catalyst candidates. Such a technique can accurately determine chemical and catalytic properties of various classes of materials: metals, alloys, or oxides and when combined with experimental screening, can reduce costs for chemicals, while being timesaving. Moreover, for less than a decade, techniques in artificial intelligence tremendously helped improve both the accuracy and speed of catalytic materials screening. Hence, in this work, the screening of heterogeneous catalysts based on our recent work will be presented, where the case of metal and high-entropy alloy catalysts will be showcased. For the metal catalysts, our screening tool – the “Ratings Concept” helps screen for reactive and stable catalysts for the CO<sub>2</sub> reforming process, while in the case of high-entropy alloy catalysts, the screening protocol of the three-way catalyst in the passive NH<sub>3</sub>-SCR process will be discussed.

**Keywords:** *Density Functional Theory (DFT), First-Principles, Gaussian Process Regression (GPR), three-way catalysts (TWC)*

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**RESEARCH INTERESTS**

Computational Catalysis Engineering  
Density Functional Theory (DFT)  
Microkinetic Modeling  
Computational Energy Materials Design  
Heterogeneous Catalysis Theory  
Materials Informatics

# A Systematic Investigation of MBene Anodes for Metal Ion Batteries: A First-Principles Study

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## Abstract

Discovering high-performance electrode materials for rechargeable metal-ion batteries has been of great importance for over the decades and remains ongoing. Transition metal borides (MBenes), a novel class of two-dimensional (2D) materials, with high surface area and intrinsic conductivity, emerge as potential candidates for this application. Due to the diversity of MBene compositions, termination groups, transition metals, and phases, a rational design of MBene-based electrodes become crucial. In our study, we therefore systematically screened various  $M_2B_2$  MBene with diverse transition metals ( $M = 3d, 4d, \text{ and } 5d$  elements) and phases (orthorhombic, hexagonal, trigonal, and tetragonal) for potential anode materials in metal-ion batteries (Li-ion, Na-ion, Mg-ion, and Al-ion). We employed periodic model calculations based on density functional theory (DFT) to assess their stabilities via cohesive energy. We explored single metal atom adsorption on  $M_2B_2$  and followed by layer-by-layer adsorption to estimate their open circuit voltage and gravimetric capacity. The energy barriers of metal diffusion on the surface were also examined. Additionally, we employed machine learning techniques to discover a descriptive model elucidating the correlation between basic  $M_2B_2$  properties and their performance. Our findings and proposed descriptors could provide insights into the metal adsorption process and theoretical guidance for development of novel MBene-based anodes.

*Keywords: Metal-ion batteries, MBene, Density functional theory, Transition metal*

# Mechanism of Glucose Electrooxidation to Gluconolactone on Gold Nanocluster Surface

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## Abstract

We develop a computational workflow for high – throughput screening of nanocluster catalyst for glucose oxidation. Our approach evaluates electrocatalytic performance of nanoclusters at thermodynamic and kinetic viewpoints. The workflow begins with randomly generating a huge number of initial conformers, then performs a massive geometry optimization to find the stable conformers of glucose on nanocluster surface. A python module is built to construct the free energy diagram based on the computational hydrogen electrode method (CHE) potential. In combination with xTB package, this module generates automatically intermediates from the stable conformers, and performs geometry optimization. We use transition state optimization of Gaussian package to find TS. Herein we present the detailed mechanism of glucose oxidation on Au<sub>147</sub> nanocluster using our computational workflow.

*Keywords: Non-Enzyme Glucose Sensor, Electrocatalyst, Nanocluster*

# First-principles study of metal-decorated biphenylene monolayer as promising hydrogen storage materials

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## Abstract

Alternative and eco-friendly fuels such as hydrogen energy play an important role in developing a sustainable and enduring society. A crucial aspect of the hydrogen economy depends on the efficiency of hydrogen storage methods. Metal-decorated carbon-containing two-dimensional monolayers have garnered attention as potential hydrogen storage materials due to their open structures, which enhance storage capacity. In this study, we conducted comprehensive first-principles calculations employing density functional theory (DFT) to assess the performance of metal-decorated biphenylene nanosheets. We screened various metal-decorated biphenylene configurations with different metal groups, including alkali metals, alkaline earth metals, as well as 3d and 4d transition metals. We examined the adsorption energy of metal-decorated biphenylene nanosheets and explored hydrogen adsorption on these structures to determine gravimetric weight percentages (wt%) and desorption temperatures for hydrogen. Additionally, we investigated the potential for metal-metal clustering, which could impact the practical utility of these materials for hydrogen storage. Our findings offer valuable insights into the potential of metal-decorated biphenylene nanosheets as hydrogen storage materials and provide theoretical guidance for their further development in this area of research.

*Keywords: Biphenylene, Hydrogen storage, Density functional theory*

## Insights into different selectivity in HMF hydrogenation over Ni and Cu catalysts through molecular simulation

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### Abstract

The 5-hydroxymethylfurfural (HMF) is one of well-known platform chemicals in bio-refinery. HMF can be used as a substrate in chemical reactions to synthesize a variety of value-added products, including 2,5-dihydroxymethylfuran (DHMF) and 2,5-dihydroxymethyltetrahydrofuran (DHMTHF). This work applied a plane wave-based density functional theory (DFT) method to examine the different selectivity of HMF hydrogenation in Ni and Cu catalysts. Possible reaction pathways in gas and solution phases were systematically investigated and compared in this work. The calculated results revealed that the competition between the third hydrogenation step and the DHMF desorption step clearly explains the different selectivity of over Ni(111) and Cu(111). The thermodynamic and kinetic analyses showed that Ni(111) prefers the DHMTHF production in range of 0 K to 373.15 K. On a Cu(111) surface, DHMTHF is the preferred product at temperatures ranging from 0 K to 188 K, while DHMF becomes favorable at elevated temperatures. At 373.15 K, the turnover frequency (TOF) values for DHMTHF over Ni(111) and DHMF over Cu(111) at 373.15 are approximated  $4.01 \times 10^5$  (h<sup>-1</sup>) and  $1.79 \times 10^3$  (h<sup>-1</sup>), respectively. Furthermore, the calculations demonstrated that in the aqueous phase, the hydrogenation of HMF over Ni(111) has high DHMF selectivity, similar to the reaction over Cu(111). For Ni, the desorption free energy of DHMF in water ( $\epsilon=78.4$ ), is 0.29 eV, which is significantly reduced compared to the 1.30 eV of the gas-phase reaction. This aspect corresponds well with experiment reported in literature.

**Keywords:** HMF hydrogenation, DFT, Ni, Cu, Mechanism



# Charge transport properties in metal halide hybrid perovskites: the perspective of large polarons, alloy scattering, and self-trapped carriers

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## Abstract

Metal halide hybrid perovskites (MHPs) have received a lot of attention in the past ten years as a result of the quick advancement of perovskite-based optoelectronic devices, such as photovoltaics and light-emitting diodes, as well as their intriguing fundamental physical properties. In MHP materials, lead-halide perovskites,  $\text{APbX}_3$ , and lead-free double perovskites,  $\text{A}_2\text{BB}'\text{X}_6$ , are state-of-the-art material systems with tunable electronic and optoelectronic properties. Herein, we develop transport models based on large polarons, alloy scattering, and self-trapped carriers to elucidate charge-carrier transport dynamics and mobilities in both lead-halide and lead-free double perovskites. Hot carriers are produced through photoexcitation and rapidly relaxed to become free charge carriers in a scattering process via LO phonon emissions. Within a subpicosecond, large polarons are formed via Fröhlich interactions between free charge carriers (both electrons and holes) and the macroscopic electric field produced by LO phonons. Large polaron transport is a band-like transport characteristic that occurs in MHPs very soon after photoexcitation. The estimated charge-carrier mobility values based on large polaron transport were  $32 \text{ cm}^2/(\text{Vs})$  in  $\text{MAPbI}_3$ ,  $28 \text{ cm}^2/(\text{Vs})$  in  $\text{FAPbI}_3$ ,  $40 \text{ cm}^2/(\text{Vs})$  in  $\text{FA}_{0.83}\text{Cs}_{0.17}\text{PbI}_3$ ,  $12 \text{ cm}^2/(\text{Vs})$  in  $\text{FAPbBr}_3$ , and  $11 \text{ cm}^2/(\text{Vs})$  in  $\text{FA}_{0.83}\text{Cs}_{0.17}\text{PbBr}_3$ , which were in very good quantitative agreement with published experimental data. The estimated mobility values in the  $11\text{--}34 \text{ cm}^2/(\text{Vs})$  range, which were derived from large polaron transport and I-Br alloy scattering, agreed well with the experimental mobility measurements of  $11\text{--}37 \text{ cm}^2/(\text{Vs})$  in  $\text{FA}_{0.83}\text{Cs}_{0.17}\text{Pb}(\text{I}_{1-x}\text{Br}_x)_3$ . While, in a lead-free  $\text{Cs}_2\text{AgBiBr}_6$  double perovskite, charge carriers are self-trapped by very strong phonon interactions within a few picoseconds, forming small polarons localized within a few unit cells, which are the so-called self-trapped carriers. This approach yielded a charge-carrier mobility of  $0.52 \text{ cm}^2/(\text{Vs})$ , which is well in line with the experimental results. These results provide new information about the dynamics of charge transport in MHPs.

**Keywords:** Metal halide hybrid perovskites, charge-carrier mobility, large polarons, alloy scattering, self-trapped carriers.

# Unraveling the role of hydrogen insertion in enhancing electrochemical performance of $V_2O_5$ cathode for Mg-ion batteries: A first-principles study

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## Abstract

Vanadium pentoxide ( $V_2O_5$ ) exhibits tremendous promise as a cathode material for Mg-ion batteries due to its impressive theoretical capacity. However, its commercial viability is hindered by issues such as sluggish electron-ion conductivity and capacity degradation over cycling. This study explores the potential of improving  $V_2O_5$  cathodes by introducing a small quantity of water into the electrolyte, which remarkably enhances charge transport kinetics and augments the cathode's capacity. While the mechanism of this enhancement has been attributed to water dissociation and the provision of hydrogen (H) for insertion into the cathode, the precise role of H insertion remains unclear. In this investigation, we employ first-principles computations to elucidate the impact of H insertion on various aspects of  $V_2O_5$ 's performance, including electronic conductivity, magnesium (Mg) diffusion kinetics, and structural stability upon Mg intercalation. Our findings reveal that high concentrations of inserted H effectively reduce the band gap and boost the electronic conductivity of  $V_2O_5$ . Furthermore, the inserted H acts as a charge carrier, thereby enhancing the cathode's capacity. Remarkably, the transport kinetics of H surpass those of Mg, suggesting that during discharge, the cathode may contain a substantial amount of pre-inserted H before Mg intercalation. The presence of pre-inserted H in the  $V_2O_5$  structure accelerates Mg diffusion by significantly lowering the diffusion barrier from 0.93 to 0.23 eV. Additionally, a fully protonated  $V_2O_5$  cathode effectively suppresses the irreversible  $\alpha$ -to- $\delta$  phase transition, a known culprit of capacity fading. These improvements in ion transport kinetics and phase transformation suppression are attributed to the weakened electrostatic interaction between Mg ions and lattice oxygen resulting from H insertion. These findings provide valuable insights for the rational design of strategies aimed at enhancing the electrochemical performance of  $V_2O_5$  cathodes in Mg-ion batteries, paving the way for more efficient and durable energy storage devices.

**Keywords:** Aqueous electrolyte,  $V_2O_5$ , first-principles calculations, Mg-ion batteries, H insertion

# Suppression of Shuttle Effect via Single Atom Deposition on Biphenylene Cathodes of Na-S Batteries: A First-Principles Study

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## Abstract

Sodium-sulfur (Na-S) batteries show promise for advanced and large-scale energy storage due to their high specific capacity and abundant raw materials. However, they still cope with several challenges such as low electrical conductivity of electrode material and polysulfide shuttling leading to capacity fading. Here, we propose a novel approach involving the decoration of transition metal (TM; Fe and Co) atoms onto a 2D conductive carbon-based material known as biphenylene (BP), to serve as a cathode material. We carried out DFT calculations to investigate the potential of TM atom decoration to suppress the shuttle effect. Our calculations reveal that TM decoration onto BP (TM@BP) enhances adsorption strength of sodium-polysulfide species (NaPS) and hinders their dissolution into the electrolytes. Furthermore, small NaPS (Na<sub>2</sub>S<sub>2</sub> and Na<sub>2</sub>S) adsorption on cathode material is commonly insulative but it becomes conductive in the case of TM@BP. The energy barrier of Na<sub>2</sub>S decomposition on TM@BP is lower than that observed on pristine BP. Our findings suggest that TM decoration on biphenylene effectively mitigates the shuttle effect and promotes the kinetics of the NaPS transformation reaction.

**Keywords:** Sodium-sulfur batteries, Biphenylene, 2D material, Density functional theory, Sodium polysulfides, Single atom catalyst

# Computational exploration of dual atom catalysts on defective graphene for hydrogen storage at liquid organic hydride

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## Abstract

Hydrogen is a clean and efficient energy carrier in various fuel-cell applications including vehicles, stationary and portable electronics, etc. However, the lack of a suitable method for storage and transportation is still a limitation of its applications. Liquid organic hydrogen carriers (LOHC) systems, in which hydrogen is bonded via covalent bonds are a potentially safe and cheap concept for H<sub>2</sub> storage. Hydrogen is stored and released through catalytic hydrogenation and dehydrogenation of organic molecules. The development of efficient and inexpensive catalysts for these reactions is still challenging. Currently, single and double-atom catalysts were widely studied as catalysts for various reactions. In this work, we will present a mechanistic study of the hydrogenation of benzene to cyclohexane over palladium dimers supported on nitrogen doping graphene surfaces (2Pd-N<sub>x</sub>-VG) investigated by the density functional theory (DFT) method. The energy profiles revealed that benzene hydrogenation to cyclohexane is kinetically and energetically favorable through 12B\*, 123B\*, and 1234B\* intermediates (The numbers represent the positions of the hydrogenated C). In addition, we found that the third hydrogenation step, i.e. the conversion of 12B\* to 123B\*, has a barrier of about 0.90 eV, making it the rate-limiting process in the present system. However, this barrier is slightly lower than the value of the rate-limiting step on Pt (111), 1.04 eV. This work not only reveals the molecular-scale phenomena of the surface reaction, but the outputs also guide the way to improve the activity of double-atom catalysts for benzene hydrogenation reaction.

*Keywords: Hydrogen storage, Dual atom catalysts, Defective graphene, Benzene hydrogenation, DFT calculation*

# DFT Insights into CO<sub>2</sub> Electrochemical Reduction on Cu-Based Catalysts: Effects of Explicit Solvent and Surface Structure on C<sub>2</sub> Product Selectivity

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## Abstract

Unraveling CO<sub>2</sub> electrochemical reduction mechanisms, particularly toward ethylene and ethanol, is crucial for enhancing CO<sub>2</sub> conversion within Carbon Capture, Utilization, and Storage (CCUS) strategies amidst the challenges posed by climate change and global warming. Using density functional theory (DFT) calculations, we investigate CO<sub>2</sub> electrochemical reduction to produce ethylene and ethanol on Cu-based catalysts, including pristine Cu(100) and bimetallic Cu-Zn surfaces. According to the simulation results, C–C couplings play a vital role in C<sub>2</sub> production. Notably, Cu(100) kinetically favors CO–CO coupling, while Cu-Zn kinetically promotes CO–CHO or CO–CH coupling. In the later stages of the reaction, the separation occurs through the significant C–O bond cleavage within the \*CH<sub>2</sub>CH<sub>2</sub>OH intermediate, resulting in the bifurcation of pathways leading to either ethylene or ethanol. Furthermore, key intermediates controlling product selectivity also emerge during the late protonation steps. Explicit solvent models were employed to elucidate the solvent effects on CO<sub>2</sub> electrochemical reduction mechanisms and product selectivity. Indeed, the solvent has a significant influence on the energetic stability of the key intermediates, thereby shaping the reaction pathways and product selectivity. This research offers more than theoretical clarity into solvent effects and catalyst structures on key intermediate stability, C–C coupling energy barriers, and C–O bond dissociation. It delivers a comprehensive reaction mechanism that furnishes valuable insights for refining ethylene and ethanol selectivity. This significant contribution enhances understanding of reaction complexity and provides guidance in tuning ethylene and ethanol selectivity.

**Keywords:** CO<sub>2</sub> electrochemical reduction, Cu-based catalysts, C–C couplings, density functional theory, solvent effect

# Computational Study of NH<sub>3</sub> Detection Using Metal-Decorated Siligene as a Work Function-Type Sensor

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## Abstract

Ammonia (NH<sub>3</sub>) is highly toxic and corrosive, so exposure to this compound can cause severe damage to both the health of living beings as well as the environment. Moreover, NH<sub>3</sub> is an excellent source of hydrogen that could play an important role in the development of the imminent economy based on green fuels such as hydrogen. For these reasons, the detection and storage of NH<sub>3</sub> are relevant issues. In recent years two-dimensional materials, such as graphene, have gained relevance since their one-atom thicknesses generate physicochemical properties totally different from their bulk counterparts. 2D SiGe with honeycomb lattice has been theoretically studied since its structural stability was predicted through theoretical calculations more than a decade ago. It is worth mentioning that the synthesis of similar nanostructures has been recently reported, pointing out that this material is worth further investigation. Density Functional Theory (DFT) is employed as a suitable method for studying adsorbate-adsorbent interactions. In this work DFT calculations were used to investigate the interactions of NH<sub>3</sub> molecules with 2D SiGe decorated with different metal atoms, including Li, Na, K, Mg, Ca, Sc, Ti, and Pd. By studying these interactions, the aim is to identify the most favorable metal atom that enables effective NH<sub>3</sub> adsorption and detection by evaluating the changes on its respective work function. Overall, the study presents an important step towards developing an efficient and cost-effective NH<sub>3</sub> sensor based on 2D nanomaterials, which could have practical applications in environmental monitoring, industrial safety, and green energy technologies.

*Keywords: 2D nanomaterials, sensing, work function, ammonia, DFT.*

# Density functional investigation of the carbonyl-ene reaction between encapsulated formaldehyde and propylene over **M**-Cu-BTC MOFs (**M** = Be, Mg, and Ca)

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## Abstract

The structure, electronic properties, and catalytic activity of bimetallic **M**-Cu-BTC paddlewheels (**M**= Be, Mg, and Ca) for carbonyl-ene reaction between formaldehyde and propylene were studied by DFT calculations (M06-L). The reaction initiates with the formaldehyde adsorption on the reactive site via its oxygen atom. The appearance of the substituted alkaline earth metals has a small effect on the adsorption of formaldehyde on the Cu center of the bimetallic paddlewheel as compared to the parent structure. The adsorption energies are calculated to be -14.1 (**Cu**-Be-BTC), -12.8 (**Cu**-Mg-BTC), -10.4 (**Cu**-Ca-BTC), and -13.4 (**Cu**-Cu-BTC) kcal mol<sup>-1</sup>, respectively. The distances between encapsulated formaldehyde and Cu atom of the active site of bimetallic paddlewheels and charge transfer are correlated with the adsorption energies. The reaction is proposed in a single step involving the proton transfer from coadsorbed propylene to formaldehyde oxygen and the C-C bond formation between two reactants, simultaneously. We found the substituted alkaline earth metals do not affect the catalytic performance of the Cu center for this reaction. The activation energy for the reaction at the Cu center is insignificantly different: (**Cu**-Cu-BTC (19.1 kcal mol<sup>-1</sup>), **Cu**-Be-BTC (19.0 kcal mol<sup>-1</sup>), **Cu**-Mg-BTC (19.8 kcal mol<sup>-1</sup>), and **Cu**-Ca-BTC (20.7 kcal mol<sup>-1</sup>)). However, we found that the adsorption of formaldehyde on the substituted metal sites increased as compared to the parent Cu-Cu-BTC. The adsorption energies are predicted to be -26.8 (**Be**-Cu-BTC), -25.2 (**Mg**-Cu-BTC), and -24.1 (**Ca**-Cu-BTC) kcal mol<sup>-1</sup>, respectively. The catalytic activity of this reaction on the substituted metal is greater than that on the Cu center. The catalytic activities are in the order **Be**-Cu-BTC (12.7 kcal mol<sup>-1</sup>) > **Mg**-Cu-BTC (14.4 kcal mol<sup>-1</sup>) ≈ **Ca**-Cu-BTC (15.0 kcal mol<sup>-1</sup>). The results could be explained by the greater electron transfer in the transition state. Among them, the Be site of the bimetallic **Be**-Cu-BTC paddlewheel is predicted as a promising candidate catalyst for encapsulating formaldehyde and catalyzing the carbonyl-ene reaction with propylene.

*Keywords: Metal-organic framework, Density functional theory, Formaldehyde, Carbonyl-ene reaction*

## Theoretical Study of Dechlorination for Groundwater Remediation using Sulfidized Nanoscale Zerovalent Iron

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### Abstract

Chlorinated ethenes are one of the most frequent soil and groundwater contaminants worldwide. Recently, Sulfide-modified Nanoscale Zerovalent Iron (S-NZVI) has been widely used in the removal of Trichloroethylene (TCE) for groundwater remediation. However, to further improve the understanding of the performance of the reactivity and selectivity of S-NZVI remains unclear. In this work, we investigated the performance of S-NZVI by study adsorption configuration and stability of chlorinated ethenes including tetrachloroethene (PCE), cis-1,2-dichloroethene (cis-DCE), and their mixtures with TCE on FeS (001) surfaces based on the density functional theory (DFT) calculation. DFT calculations show the possible molecular structures, surface properties and absorption properties of sulfidation.

*Keywords: Dechlorination, DFT, Sulfidized Nanoscale Zerovalent Iron, Groundwater Remediation*



# The theoretical study on ethanol synthesis catalyzed by synergistic effect of metal and non-metal dope on Graphyne

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## Abstract

The reducing of the CO<sub>2</sub> emission has been an issue for us nowadays. CO<sub>2</sub> conversion using electrocatalysis is one of the promising strategies in turning waste into valuable product. The limitation of the experiment through screening toward the high-performance catalysts in terms of cost and time have become a bottleneck, where the theoretical study could serve as a guideline for the screening. Various dual atom catalysts (DACs) have been proposed. However, the performance toward C<sub>2+</sub> products as well as the synthesizability are still not significant.

In this study, we proposed a new d-p orbital type active center consists of metal and non-metal to replace the conventional d-d orbital type dual-metal DACs, to realize the more flexible active sites. Using the B-, N-modified graphyne (GRY) as a platform for metal embedding, we compared the CO<sub>2</sub> reduction performance across various types of design surfaces. We found that Co embedded B doped graphyne is the most suitable platform for the reaction toward CC coupling and toward ethanol synthesis with low limiting potential. The synergistic effect of the Co and B-modified acetylenic linker of GRY behaves like a dual active center in conventional DACs, though the more flexible and the more delocalization of the electronic states were found in our proposed system. The performance of the catalyst can be rationalized by the charge transfer feasibility, electrostatic stabilization of the intermediates, and the increasing of the electronic states near the Fermi level which provides the more flexible intermediate binding. We hope that our new proposed d-p type active center would provide a new insight into the catalyst design of CO<sub>2</sub> reduction.

*Keywords: CO<sub>2</sub> reduction, CC coupling, C<sub>2+</sub> product, ethanol synthesis*

## Nanosafety - Excessive data, huge uncertainty How reasonable databases can solve this Gordian knot

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### Abstract

Scientists have been producing data on the safety of nanomaterials for at least three decades. At great expense and many hundreds of millions of euros/dollars, projects that address the safety of these materials to humans and the environment are funded. In the process, the trail of publications often gets lost in the confusion of the data produced, so it is often unclear whether the result is now critical and safety-relevant or purely mechanistic data. Therefore, two things must be considered when data from scientific publications are used for a safety assessment: Have the studies been conducted according to the basic principles of good laboratory or scientific practice? If so, the data are thus comprehensible because all necessary information about the material or the biological test system was provided. Furthermore, was the study performed according to the rules of toxicology by using standardized methods (e.g., OECD Guidelines) or harmonized protocols? These are important aspects of FAIR data<sup>1</sup>. Unfortunately, the quality of most studies from the last two decades is considerably below the level of good toxicological work, so that for integrating the data into a database for risk assessment, the quality according to toxicological criteria must necessarily be included and considered when drawing conclusions from the data as it has been applied by the DaNa Internet platform (<https://nanopartikel.info/en/knowledge/literature-criteria-checklist/>) for more than ten years.

This was attempted in the newly established CoCoN<sup>®</sup> database<sup>2</sup>, which uses a large number of data sets to enable certain materials to be classified according to their properties and their safety-relevant effects to be recorded and assessed at an early stage. The database is aimed at regulators, industry and scientists simultaneously and is intended to provide a basis for the safe application of new innovative materials, such as nanomaterials.

For future publications, it would be highly desirable if the data were FINDABLE and REUSABLE according to the FAIR principles. This would mean that the important information on the materials studied, the biological test models and the methods used should be included in a machine-readable version of each publication as a supplement which would lead to a great facilitation of the integration of data in databases such as CoCoN<sup>®</sup> and which would imply the solution of the Gordian knot of hazard assessment.

*Keywords: Nanosafety, COCON database, hazard assessment, study quality, FAIR data*

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<sup>1</sup> FAIR: Findable, Accessible, Interoperable, and Reusable

<sup>2</sup> CoCoN: Collection of Controlled Nanosafety Data

**Short Bio: Harald Krug**

Harald F. Krug is retired since 10/2017 from his position as Manager for the International Research Cooperations in the General Management of Empa – Swiss Laboratories for Materials Science & Technology in Switzerland (St. Gallen). Until May 2014 he was a member of the board of directors of Empa and head of the research focus area „Health&Performance“. With the founding of his own company in February 2014 he follows the rules of the ETH-Area and left the board of directors. His company NanoCASE GmbH focusses on education and consulting of manufacturing companies on the safe production and use of nanomaterials or nanomaterial-containing products. He was further appointed as Professor at the University of Berne since August 2008 and is emeritus now. His actual work with his company is focused on applications and implications of new materials, especially nanomaterials. Special emphasis lays on the reliability of published data and the generation of usable knowledge in international consortia. In projects funded by the OECD, the German and the Swiss government he established several databases presenting reliable data on nanosafety in the web. His work was awarded in 2006 with the cwi-Award of the German Ceramic Society, in 2007 with the Research Award for „Alternatives for Animal Testing“ of the State Parliament of Baden-Württemberg and in 2015, 2017, and 2020 with best oral contribution awards at the WING, EuroNanoForum, and the Nanotoxicology conferences.

Until 2009 he was the speaker of the “NanoCare“ consortium (2006-2009) and his former lab is involved in several EU-funded projects, one of which is the “European Graphene-Flagship Project”, as well as more than 10 further projects funded by different national and international funding agencies. Additionally, he is founder member of the International Alliance for Nano-EHS-Harmonization (IANH) which is engaged in the evaluation of methods for nanomaterials testing. He consults the ministries of three different European countries and is member of various advisory boards of international projects and well-known institutes and activities such as CAATEU and GENSUISSE. In 2013 he was visiting professor at the NANOTEC-Institute in Bangkok (Thailand). Since 2014 until 2017 he was the representative of Empa as Co-Editor-in-Chief for the Journal Science and Technology of Advanced Materials (STAM), which is published together with the Japanese NIMS.

Harald Krug studied Chemistry and Biology. He received his Ph.D. from the Georg-August University in Göttingen for his work in animal physiology. After a postdoc period at the Helmholtz Centre Munich, he took over the Department for Environmental Toxicology at the Karlsruhe Institute of Technology. He habilitated in 1996 in “Environmental Toxicology” at the University of Karlsruhe and got his APL Professorship in 2005. Since 2007, he has taught at the University Berne.

# The Possible Role of Autophagy in Nanomaterials Safety Assessment-Related Alternative Testing Strategies: Take the Ag/ZnO NPs for example

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## Abstract

Nanotechnology has rapidly promoted the development of a new generation of industrial and commercial products; however, it has also raised some concerns about human health and safety. To evaluate the toxicity of nanomaterials (NMs) in the traditional manner, a tremendous number of safety assessments and a large number of animals are required. For this reason, it is necessary to consider the use of alternative testing strategies that reduce, refine, or replace (3Rs) the use of animals for assessing the toxicity of NMs. Autophagy is considered an early indicator of NM interactions with cells and has been recently recognized as an important form of cell death in nanoparticle-induced toxicity. Impairment of autophagy is related to the accelerated pathogenesis of diseases. By using mechanism-based high-throughput screening in vitro, we can predict the NMs that may lead to the generation of disease outcomes in vivo. Thus, a tiered testing strategy is suggested that includes a set of standardized assays in relevant human cell lines followed by critical validation studies carried out in animals or whole organism models such as zebrafish (*Danio rerio*) for improved screening of NM safety. A thorough understanding of the mechanisms by which NMs perturb biological systems, including autophagy induction, is critical for a more comprehensive elucidation of nanotoxicity. A more profound understanding of toxicity mechanisms will also facilitate the development of prevention and intervention policies against adverse outcomes induced by NMs. The development of a tiered testing strategy for NM hazard assessment not only promotes a more widespread adoption of non-rodent or 3R principles but also makes nanotoxicology testing more ethical, relevant, and cost- and time-efficient.

**Short Bio:**

**Ying-Jan Wang,**

Ph. D. Distinguished Professor  
Department of Environmental and Occupational Health,  
College of Medicine, National Cheng Kung University



**Speaker Biographies :**

Ying-Jan Wang, Ph. D., graduated from Department of Biochemistry, National Taiwan University, College of Medicine, Taipei, Taiwan. Currently served as a distinguished professor in Department of Environmental and Occupational Health, National Cheng Kung University, College of Medical, Tainan, Taiwan. The major research focus of my laboratory is to understand the molecular mechanisms responsible for nanomaterials-triggered toxicity, and also carcinogenesis/cancer therapy. I am especially interested in elucidating the role of autophagy in regulating diverse biological processes, such as proliferation, programmed cell death, inflammation, thereby contribute to cytotoxicity, and cancer therapy. In general, basal autophagy helps maintain homeostasis, while additional autophagy is induced in response to many different forms of stress. Thus, I am enthusiastic in exploring whether autophagy acts as a pro-survival or pro-death player in toxic response of nanomaterials or during cancer therapy. By revealing the regulation pathways of autophagy, our research may help to the development of alternative testing strategies of nanotoxicology and also the effective preventive strategy to combat diseases.

## Towards Responsible Innovation: Challenges for Future Nanotechnology and Advanced Materials

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### Abstract

When dealing with novel materials and products, health and environmental impacts, ethical aspects, risk assessment and risk management, and standardization should be considered as international issues. Emerging technologies such as nanotechnology and advanced nanomaterials may have novel properties due to their nanostructures that are different from conventional materials, and need to be properly assessed and managed as unknowns. Categorizing nanomaterials relies not solely on composition, but also on various influencing factors such as size, shape, and surface state. Scientific characterization requires significant time, funding, and equipment, fostering collaboration among global industry, government, and academia.

It is important to ensure scientific reproducibility and medical/epidemiological evaluation in establishing of risk assessment methods and risk management methods. Furthermore, there are various issues from the perspective of "responsible research and innovation (RRI)", including the development of a knowledge base for assessment findings, the establishment of a system for providing information and a communication framework to society, a system for utilizing such information in industry and society, and formulating consensus-building and decision-making mechanisms. Thus, there are two approaches: one from the scientific aspect of environment, health, and safety (EHS) and the other from the ethical, legal, and social issues aspect (ELSI).

In recent years, regulations and guidelines are being developed at the national and international levels in response to the increasing commercialization of products using nanomaterials and the situation of micro- and nano-plastic dispersion in the oceans. It is also noteworthy that the European Commission has updated its recommendation on the definition of nanomaterials in 2022. Responding to these trends, Japanese industries and national institutions dealing with nanomaterials are adapting. In order to properly manage the risks associated with useful technologies and advanced materials, and to ensure that society can widely reap the benefits of such technologies and materials, it is essential that products be distributed in a healthy global market. In this context, international standardization holds significance across terminology, evaluation test methods, and risk assessment methods.

This presentation will provide an overview of the aforementioned trends in nano-safety and standards, highlighting Japan's contributions. We will then discuss issues for RRI into the future.



**Short Bio:** Toshiki NAGANO ,MBA

#### **Affiliation**

- (1) Fellow/Director of Center for Research and Development Strategy (CRDS), Japan Science and Technology Agency (JST),
- (2) Program Officer of Advanced Research Infrastructure for Materials and Nanotechnology in Japan (ARIM), Ministry of Education, Culture, Sports, Science and Technology (MEXT).

#### **Education**

B.A. in Physical Chemistry, Gakushuin University (2003, JAPAN).  
MBA. Graduate School of Management, GLOBIS University (2013, JAPAN).

#### **Professional Experience**

R&D Strategist of Nanotechnology/Advanced Materials fields in Japan, at the Think Tank Division of JST, a Japanese funding agency, since 2006. Developing strategies not only for major R&D programs, but also for an effective funding system and management that promotes interdisciplinary collaboration among government, academia, and industry sectors. Majors are physical chemistry and business management.

The other, Program Officer (PO) of the "Advanced Research Infrastructure for Materials and Nanotechnology in Japan (ARIM)" from 2021. ARIM is the successor to "Nanotechnology Platform Japan (NPF)", a research infrastructure platform covering all of Japan. ARIM and NPF are the programs of MEXT. It establishes a reliable research infrastructure platform and network for innovation through the alliance of institutes that have advanced equipment and research expertise. It is promoted for any of the researchers from young to industrial to do the share-use of the facilities, and to provide the shortest way to solve the urgent problems in science and technology. 25 National Institutes and Universities are united and establish a single structure for "Cutting-Edge Common Users Facility for Nanotechnology and Advanced Materials". In addition to sharing advanced facilities, ARIM supports data-driven research for a wide range of users by structuring the vast amount of materials research data generated by the use of shared facilities and providing it as a data infrastructure.

Website: (1) <https://www.jst.go.jp/crds/index.html>, (2) <https://nanonet.mext.go.jp/>

## Activities of Center for NanoSafety Metrology in Korea

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### Abstract

Nanotechnology is no longer a field in its primary age. This field has now entered a maturing period, as reflected by the generous use of the term “Nano” in our everyday lives and the seemingly endless number of products professing to make use of this technology. It is important, then, that the nano-products and nano-application will be guided or even modified to ensure that the appropriate safety steps are taken. For systematic and efficient technical supports for domestic and global nanosafety issues and concerns, the Korea Government (Ministry of Science and ICT) established the Nanosafety Metrology Center at KRISS on 1<sup>st</sup> May, 2014 for a 10 year-project. We are tasked with establishing standards with traceability for nanosafety evaluation, preparing and disseminating certified reference nanomaterials (CRMs), implementing international comparison studies to build up standards, and supporting the establishment of a national nanosafety database. In this talk, recent activities including CRMs and SOPs developed in KRISS, ISO documents, and international collaborations for nanosafety will be presented.

*Keywords: Nanotechnology, Nanosafety, CRM, standards, nanosafety database*



### **Short Bio:**

#### **Dr. Jaeseok Kim**

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### **EDUCATION**

Gwangju Institute of Science and Technology  
PhD Environmental engineering 2012  
Chonnam National University  
MS Mechanical engineering 2006  
Chonnam National University  
BS Automotive engineering 2004

### **PROFESSIONAL ACTIVITIES**

Principle research scientist (2017-Present), Korea Research Institute of Standards and Science, Daejeon, Korea  
Post-doc fellow (2015-2017), Korea Polar Research Institute, Incheon, Korea  
Post-doc fellow (2012-2015), University of Eastern Finland, Kuopio, Finland

### **MAIN SCIENTIFIC PUBLICATION**

- 1.J. Yoo, S.M. Lee, K. Lee, S.C. Lim, M.S. Jeong, J. Kim and T.G. Lee (2023) Functional group inhomogeneity in graphene oxide using correlative absorption spectroscopy, Appl. Surf. Sci., 613, 155885.
- 2.C. Minelli,....., J. Kim.... et al. (2022), Versailles project on advanced materials and standards (VAMAS) interlaboratory study on measuring the number concentration of colloidal gold nanoparticles, Nanoscale, 14(12), 4690-4704.
- 3.I.Y. Kim, J.W. Choi, I.H. Kwon, S. Hwangbo, S.H. Bae, M. Kwak, J. Kim, T.G. Lee and M.B. Heo (2022), Variations in in vitro toxicity of silica nanoparticles according to scaffold type in a 3D culture system using a micropillar/microwell chip platform, Sens. Actuato B-Chem., 369.
- 4.S.A. Hwangbo, M. Kwak, J. Kim, and T.G. Lee (2021), Novel surfactant-free water dispersion technique of TiO<sub>2</sub> NPS using focused ultrasound system, Nanomaterials, 11(2), 1-15.
- 5.J. Park, M. Kwak, N.W. Song, and J. Kim (2020), Effect of colloidal nanoparticle concentration on sizing analysis with an electrospray scanning mobility particle sizer, Appl. Nanosci., 10(1), 329-336.

### **RESEARCH INTERESTS**

His general research interest is to develop SOPs for measuring size and number concentration of nanoparticles using various instruments. To understand size and number concentration of nanoparticles in nano-products he is using ES-SMPS (electrospray scanning mobility particle sizer), NTA (nanoparticle tracking analyzer), and sp-ICP-MS techniques.

## Insights From Physical-Chemical Testing in Nano-Based Products

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### Abstract

Nanotechnology has gradually but profoundly made its mark across various global industries. This rapid pace of technological revolution is particularly evident in the developed world, where nano-scale markets have swiftly risen to prominence in the past decade. According to Marina et.al, most of the products (71%) lack sufficient supporting information to confirm the use of nanomaterials, casting doubt on the validity of the claim. Additionally, in a report jointly produced by the United Nations Environment Programme and the World Health Organization, known as the Strategic Approach to International Chemicals Management (SAICM), concerns have arisen regarding the potential risks posed to human health and the environment by nanotechnologies and manufactured nanomaterials. The intricacies of physical-chemical testing, shedding light on how these tests can be used to uncover fundamental properties such as nanoparticle size and surface morphology. Real-world case studies of nano-based products readily available locally can provide clear examples how these testing directly impact product development processes. Thus, the goal of this testing is to establish nanotechnology as a prominent technology driver for the nation, while concurrently enhancing stakeholder awareness of the health and safety implications associated with nano-based products.

*Keywords: Proteomics, adverse outcome pathway, nanoplastics, microplastics, intestinal model*

**Short Bio:**

Dominic Geruka, a graduate student in chemistry, received his Diploma in Science and Bachelor of Science (Honours) in Chemistry from Mara University of Technology in 2013 and 2016, respectively. In 2016, he joined the Clinical Research Centre at Sarawak General Hospital (CRC, SGH) as a research officer.

During his 3-year tenure at CRC SGH, he obtained Good Clinical Practice (GCP) accreditation and served as one of the authorized signatories for the laboratory. The CRC SGH laboratory is certified in MS ISO 17025 and MS ISO 15189, allowing him to actively participate in clinical trials from Phase 1 to Bioequivalence Studies as a clinical laboratory assistant. Additionally, he successfully coordinated several investigators-initiated trials as a co-PI.

In January 2020, he furthered his career as an Assistant Director at the National Nanotechnology Centre (NNC) under the Ministry of Science, Technology & Innovation. Currently, he is responsible for supporting a major nano safety project while ensuring the smooth operation of the regulatory section on a daily basis at NNC.

ChM Dominic Geruka  
Assistant Director & Research Officer  
National Nanotechnology Centre (NNC),  
Ministry of Science, Technology &  
Innovation (MOSTI)



## Using proteomic approach for investigation of adverse outcome pathways related to nano- and microplastics in human 3D-intestinal model

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<sup>b</sup>National Center for Genetic Engineering and Biotechnology (BIOTEC), National Science and Technology Development Agency (NSTDA), Pathum Thani, Thailand

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### Abstract

Plastics can be found in food packaging, shopping bag, household items, such as toothbrushes and pens, and facial cleansers. Nanoplastics can be produced by fragmentation or dissociation of microplastic debris. As a result of the widespread use of plastics, human body is exposed to nanoplastics by inhalation, percutaneous or by foods. Microplastics are frequently detected in the gastrointestinal tract of marine animals. Recently, there was the reports of the biodistribution of microplastics in human blood and excretion of microplastics in human stool. However, there are limited numbers of studies regarding the effect of nanoparticles on human health. Since gastrointestinal system is the primary barrier to expose with nanoplastics in contaminated foods, this study therefore aimed to investigate the human health impact of nanoplastics using human 3D-intestinal model. In this study, proteomic approach was used to investigate the adverse outcomes pathways related to nano- and microplastics in human 3D-intestinal model after single exposure (4 h) and repeated exposure (4 h exposure daily for 7 days). The representative nanoplastics and microplastics used in this study includes polystyrene (PS) and polyethylene terephthalate (PET). Our results suggest that all particles tested (PS and PET) did not decrease tissue viability of human 3D-intestinal model after single exposure and repeated exposure. However, our results suggest that repeated exposure of PET (140 nm) induced inflammatory cytokine release. We further investigated the biodistribution of PS and PET in 3D-intestinal model. Our results indicated the intestinal tissue uptake of PS and PET in nanosize (30 nm, 100 nm, 200 nm, 450 nm), whereas no tissue uptake and accumulation of PS 1.8  $\mu$ m after 4 h exposure was observed. Results from proteomic analysis indicated that the most common pathways involving in the adverse outcome pathway of single and repeated exposure of PET 140 nm, PS 100 nm and PS 1.8  $\mu$ m in 3D-intestinal model are inflammation mediated by cytokine and cytokine signaling pathway, integrin signaling pathway, Wnt signaling pathway, Huntington disease, heterotrimeric G-protein signaling pathway-GI alpha and Gs alpha mediated pathway and the gonadotropin-releasing hormone receptor pathway. Our results would be the supporting evidence to deeply explain the toxicity of nano- and microplastics on gastrointestinal system and adverse outcome pathways of nano- and microplastics on human health.

*Keywords: Proteomics, adverse outcome pathway, nanoplastics, microplastics, intestinal model*

**Short Bio:**

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**Education:**

April 2007 – March 2010:

Doctor of Philosophy (Pharmaceutical Sciences, Pharmacokinetics/metabolism),  
Graduate School of Pharmaceutical Sciences, Chiba University, Chiba, Japan

April 2005 – March 2007:

Master of Pharmaceutical Sciences (Biochemical Pharmacology and Biototoxicology),  
Graduate School of Pharmaceutical Sciences, Chiba University, Chiba, Japan

May 1997 – March 2002:

Bachelor of Science in Pharmacy, Chulalongkorn University (First class honours)

**Fields of specialize:**

Nanotoxicology, Molecular toxicology, Predictive model for toxicology, 3D-tissue model

**Work experience:**

February 2019 – present:

Research Team Leader, Nano Safety and Bioactivity Research Team, National Nanotechnology Center,  
National Science and Technology Development Agency

April 2010 – January 2019:

Researcher, Nano Safety and Risk Assessment Laboratory, National Nanotechnology Center, National  
Science and Technology Development Agency

April 2002 – March 2004:

Lecturer, Bachelor degree's course, Department of Biopharmacy, Faculty of Pharmaceutical Sciences,  
Srinakharinwirot University

**Research Interest/ Work Experience**

Currently, my research focus under the Nano Environmental and Health Safety Research Team is aimed at the development of an advanced predictive model especially on nanotoxicology and efficacy evaluation. The toxicity and adverse outcome pathway related to ultrafine particles (UFPs), nanoplastics and engineered nanoparticles were investigated using the in vitro cells and 3D-tissue-based model and omics approaches.

**International committee/reviewer:**

Reviewer of Toxicological Letter  
Reviewer of Scientific Reports

**Active Membership**

European Society of Alternatives to Animal Testing  
Thai Society of Toxicology

## Dynamic Cellular Effects of Airborne Nanoparticles (PM<sub>0.1</sub>) in Upper Southeast Asia via High-Speed Scanning Ion Conductance Microscopy

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### Abstract

Air pollution, especially from particulate matter (PM), is one of the major environmental issues in Southeast Asia. Size-fractionated PM is the most important because different particle sizes can penetrate different human respiratory tracts and organ systems. This study aims to evaluate how size-fractionated PM down to PM<sub>0.1</sub> affects cellular dynamics via High-Speed Scanning Ion Conductance Microscopy (HS-SICM). The ambient PMs were collected from upper southeast Asian countries during a biomass burning episode. In each size fraction, chemical compositions were evaluated, i.e., organic and elemental carbon. Single particle sizes were analyzed by scanning electron microscopy (SEM) and sizes of PM<sub>0.1</sub>, PM<sub>0.1-0.5</sub>, PM<sub>0.5-1.0</sub>, and PM<sub>1.0-2.5</sub> particles dispersed in pure water were analyzed by Zetasizer Nano instrument. The cell toxicity experiments were performed by adding four different particle solutions to the cell medium. Two commonly used cell types, HeLa and Cos-7, were examined. A handmade tip-scan-type high-speed SICM was used to create the topographic images and associated mechanical mapping images of HeLa cells. HS-SICM for showing the physical characteristics of live cells after PM<sub>x</sub> particle uptake. The outcomes demonstrated that cell membranes could easily wrap and ingest PM<sub>0.1</sub> and PM<sub>0.1-0.5</sub> particles. At the immediate surfaces of live cells, PM<sub>0.1</sub> and PM<sub>0.1-0.5</sub> particles may be internally absorbed simultaneously. The results show that PM<sub>0.1</sub> and PM<sub>0.1-0.5</sub> particles underwent considerable morphological changes, whereas PM<sub>0.5-1.0</sub> and PM<sub>1.0-2.5</sub> particles underwent essentially minimal morphological changes. Therefore, the interactions between living human cells and ambient PMs have been visualized using HS-SICM. In order to examine cell-PM interactions, this study takes into account the most recent in vitro impacts of air pollutants and how they might be questioned. The findings can be used to better understand how airborne PM pollution affects human health and to create better mitigation strategies.

**Keywords:** PM<sub>0.1</sub>, Thailand, Health effects, Biomass burning, HS-SICM

**Short Bio: Worradorn Phairuang (Ph.D.)**

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Kanazawa University, Kakuma Machi, Kanazawa, Ishikawa, 920-1192, Japan



**EDUCATION BACKGROUND**

- |           |   |
|-----------|---|
| 2013-2016 | Doctor of Philosophy (Environmental Science and Engineering)<br>Graduate School of Natural Science and Technology, Kanazawa University, Japan                 |
| 2012-2013 | Research Student (Atmospheric Environment and Pollution Control Engineering)<br>Graduate School of Natural Science and Technology, Kanazawa University, Japan |
| 2008-2011 | Master of Science (Biology) GPA 3.80/4.00<br>Concentration in Ecology and Environment, Chiang Mai University, Thailand  |
| 2004-2008 | Bachelor of Science (Biology) GPA 3.59/4.00 (First Class Honors)<br>Concentration in Plant Science and Technology, Chiang Mai University, Thailand            |

**WORK EXPERIENCES**

- 2022-05 – present Assistant Professor, Faculty of Geosciences and Civil Engineering, Kanazawa University, Japan  
2020.10 - 2022.04 Lecturer, Department of Geography, Faculty of Social Sciences, Chiang Mai University, Thailand  
2016.08 - 2020.09 Lecturer, Faculty of Environmental Management, Prince of Songkla University, Thailand

**RESEARCH INTEREST**

Atmospheric Sciences, Earth Observation data, Machine learning, Nanoparticles (PM0.1), Health Effects

**SCHOLARSHIPS and AWARDS**

- |            |   |
|------------|---|
| 2020.3     | Excellent Researcher Award, Faculty of Environmental Management,<br>Prince of Songkla University, Thailand                            |
| 2019.11-12 | Bilateral Joint Research Projects between Japan and Thailand, Kanazawa University,<br>Japan (JSPS-NRCT)                               |
| 2019.6     | ASEA-UNINET Staff Exchange, University of Vienna, Austria   |
| 2019.1-3   | Follow-up Research Fellowship, Kanazawa University, Japan (JASSO)   |
| 2018.4-6   | Post-Doctoral Fellowship (Aerosol Physics and Environmental Physics), University of Vienna,<br>Austria (Ernst Mach Grant-ASEA-UNINET) |
| 2012-2016  | Japanese Government Scholarship, Japan (Monbukagakusho)   |
| 2009-2011  | Graduated Fellowship from Biodiversity Research and Training Program, Thailand (BRT)  |
| 2007.4     | The Best Student Award in 15th Marine Ecology Summer Course 2007 at Phuket Marine<br>Biological Center, Thailand (PMBC)               |
| 2001-2011  | Development and Promotion of Science and Technology Talent Project, Thailand (DPST)   |

## Particle size distribution, morphology and elemental composition of ultrafine particles in Bangkok traffic area comparing to Euro4 diesel exhaust particles

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<sup>g</sup>Research Unit: HAUS IAQ, Chulalongkorn University Bangkok 10330, Thailand

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### Abstract

Ultrafine particles (UFPs), or PM<sub>0.1</sub>, raise health concerns due to their ability to deeply penetrate the respiratory system, potentially carrying toxins that induce inflammation and damage to lung tissues, affecting other organs. UFPs mainly originate from fossil fuel and diesel combustion, posing a significant concern in urban areas, particularly those near major roads like Bangkok, known for heavy traffic congestion and a high volume of vehicles. Most UFPs mass from exhaust engines consists of carbonaceous materials, organic compounds, trace metal oxides, sulfates, nitrate ions, and PAHs. However, there is limited information of particle size distribution, morphology and elemental composition of UFPs in Bangkok traffic area and their relation to human health. Therefore, this study aimed to characterize the size distribution and major chemical compositions of ambient air in Bangkok's traffic areas during haze episodes on January to May 2021. It conducted comparisons with Euro4 diesel exhaust particles collected from the PCD's automotive emission laboratory using a nanosampler. Collected ambient air particles (n=35) exhibit average mass fractions as follows: PM<sub>>10 μm</sub> (22%), PM<sub>2.5-10 μm</sub> (28%), PM<sub>1-2.5 μm</sub> (14%), PM<sub>0.5-1 μm</sub> (17%), PM<sub>0.1-0.5 μm</sub> (10%), and PM<sub><0.1 μm</sub> (9%). Conversely, Euro4 diesel exhaust particles (n=30) show different mass fractions in the corresponding size categories: 7%, 9%, 12%, 15%, 14%, and 43%. UFPs in ambient air had a lower fraction of PM<sub><0.1 μm</sub> compared to diesel exhaust, suggesting a greater health risk from the latter. Scanning electron microscopy (SEM) revealed similar particle shapes in both ambient air and diesel exhaust, suggesting combustion and vehicle emissions as sources. Chemical analysis showed the presence of Si, S, and C, consistent with combustion-related pollutants. Understanding UFPs composition is vital for source identification, mitigation, and community health protection. Further research is needed to explore the health implications of varying UFP compositions in specific areas.

**Keywords:** Ultrafine particles, Particle size distribution, Nanosampler, Bangkok traffic, Diesel exhaust particle



## Effect of biodiesel concentrations on particulate emissions from the combustion of biodiesel generated by Euro 2 vehicle: Concentrations, size distributions and carbonaceous components

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### Abstract

More than 90% of vehicular exhausts come from diesel engines, which emit PM<sub>2.5</sub>, a major global air pollutant. Currently, diesel fuels in Thailand are a mixture of petroleum diesel and biodiesel, with the ratio of 7%/93% (B7), 10%/90% (B10), and 20%/80% (B20). Despite an extensive use of biodiesel in Thailand, the influence of biodiesel concentration on the carbon components of the particulate emissions is not well understood. This project aims to investigate the effects of biodiesel fractions on the mass concentrations, size distributions, and carbonaceous components of the size-segregated diesel exhaust particles down to 0.1  $\mu\text{m}$ . The biodiesel blend used in this study contained biodiesel at the concentrations of 7%, 10%, 20%, and 30%. The experiments were performed on a chassis dynamometer using a Euro 2 light-duty car. The size-segregated diesel exhaust particles were collected using a NanoSampler, which was connected to an exhaust tunnel of the testing system. Moreover, emissions during the driving pattern specific to traffic areas in Bangkok were compared to those during the New European Driving Cycle (NEDC). Mass concentrations and size distribution were determined using the gravimetric method. Carbonaceous components including organic carbon (OC, light-reflecting) and elemental carbon (EC, light-absorbing) of the samples were analyzed using the thermal optical reflectance ('IMPROVE' protocol). The understanding of OC and EC size distribution, and the corresponding OC/EC ratio, provides insight into the contribution of biodiesel emissions towards greenhouse effect.

**Keywords:** Biodiesel, Air pollution, Diesel exhaust particles, Organic carbon, Elemental carbon

## Application of lung tissue model for study the adverse outcome pathways of ultrafine particles and fine particles in Bangkok traffic area

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### Abstract

One major air pollutants is PM 2.5, defined as particles with a diameter of 2.5  $\mu\text{m}$  or less. High concentrations of ultrafine particles (UFPs) are harmful to human health, especially the lungs leading to coughing, worsen asthma, systemic inflammation, and other potential health issues such as cancer. However, limited research exists on their effects, and the mechanisms behind UFPs and fine particles' impact on lung health remain unclear. Therefore, this project aims to apply a lung tissue model for study the adverse outcome pathways (AOPs) of UFPs ( $< 0.1 \mu\text{m}$ , PM<sub>0.1</sub>) and fine particles (PM<sub>1-2.5</sub>  $\mu\text{m}$ ) in Bangkok traffic area. Lung tissue models derived from primary cells, labeled with epithelial cellular adhesion molecule, were cultured on transwells under air-liquid interface culture for 20 days and applied to study the AOPs of UFPs and fine particles. The developed lung tissue models exhibit expression of aquaporin 3, cytokeratin-8, lysophosphatidylcholine acyltransferase, mucin 5AC, surfactant protein B, and pro-surfactant protein C. The results indicated that PM<sub>0.1</sub> and PM<sub>1-2.5</sub>  $\mu\text{m}$  did not cause acute toxicity in lung tissue models but altered protein expression. Protein change after UFPs and fines exposure in lung tissue model was analyzed by proteomic approach to link with adverse effect outcomes of UFPs. The significantly up- and down-regulated proteins from ambient and Euro4 diesel exhaust particles treated cells demonstrated the numbers of commonly expressed proteins higher than diesel treated cells. In addition, Up- and down-regulated proteins of PM<sub>0.1</sub> and PM<sub>1-2.5</sub>  $\mu\text{m}$  treated cells showed similar pathways including Integrin signaling pathway, FGF signaling pathway, Inflammation mediated by chemokine and cytokine signaling pathway, and EGF receptor signaling pathway. Our results suggest that the developed lung tissue models can be effectively applied to study the toxicity and adverse effects of PM and other environment toxicants for health risk assessment.

*Keywords: lung tissue model; adverse effect outcomes; ultrafine particles; fine particles; proteomics*

## The safety study of intestinal exposure to food-grade titanium dioxide (E171) using 3D-intestinal model

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### Abstract

Food-grade titanium dioxide (E171) is one of the most used food additives for whitening and brightening in food industry. The Food and Drug Administration of the United States allowed the use of food-grade E171 with a titanium dioxide (TiO<sub>2</sub>) level in food-weight limitation. However, the widespread usage of E171 in daily foods has increased, resulting in a high TiO<sub>2</sub> exposure level in the body. The intestinal barrier keeps hazardous substances out of the small intestine while allowing nutrients from food to pass through. The presence of a high nano-sized fraction of E171 may alter the gut barrier and change its homeostatic function. In this study, a 3D intestinal model is used to examine how food-grade E171 affects cytotoxicity and inflammation in the human small intestine. E171 was exposed on the 3D intestinal model for single and repeated treatment mimic the daily exposure in the small intestine. Then, the cytotoxic and inflammatory effects on 3D intestinal model were determined by MTT and cytokine releases, respectively. In addition, protein analysis and genotoxicity testing were also investigated using proteomic approach and comet assay. The concentration of E171 at 10 and 100 µg/mL for single treatment for 4 h in 3D intestinal model showed the non-significant cytotoxicity. However, the repeated treatment (4 h a day for 14 days) of E171 at 10 and 100 µg/mL demonstrated the increasing of DNA damage in 3D-intestinal model. Furthermore, the result of proteomic analysis at 10 µg/mL illustrated the alteration of protein expression profile of inflammatory and stress-related pathway. The effect of repeated treatment of E171 at 10 µg/mL on 3D intestinal model revealed the elevated hazard comparing to the non-treatment and single exposure of E171 due to the cumulative toxicity of E171. These data support the health risk assessment of the excessive and continuous oral intake of E171 from dietary foods.

**Keywords:** Food-grade titanium dioxide (E171), 3D intestinal model, inflammation, genotoxicity, proteomic

# Flexible Electronics: Challenges and Opportunities — a Materials Science View

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## Abstract

In recent years, immense efforts in the flexible electronics field have led to unprecedented progress and to devices of ever increasing performance. Despite these advances, new opportunities are sought in order to widen the applications of organic-based technologies and expand their functionalities and features. We discuss here challenges and opportunities, with focus on the use of multicomponent systems for, e.g., increasing the mechanical flexibility and stability of organic electronic products, or introducing other features such as self-encapsulation and faster mixed ion-electron transport. One specific strategy is based on blending polymeric insulators with organic semiconductors; which has led to a desired improvement of the mechanical properties of organic devices, producing in certain scenarios robust and stable architectures. Here we discuss the working principle of semiconductor:insulator blends, examining the different approaches that have recently been reported in literature. We illustrate how organic field-effect transistors (OFET)s and organic solar cells (OPV)s can be fabricated with such systems without detrimental effects on the resulting device characteristics even at high contents of the insulator. Furthermore, we review how blending can assist in the fabrication of more reliable and versatile organic electrochemical transistors (OECT)s.

**Short Bio: Natalie Stingelin**

Natalie Stingelin is a Full Professor at the Georgia Institute of Technology and the Chair of the School of Materials Science & Engineering. She held prior positions at Imperial College London, UK, at Queen Mary University of London, UK; the Philips Research Laboratories in Eindhoven, The Netherlands; the Cavendish Laboratories, University of Cambridge, UK; and the Swiss Federal Institute of Technology (ETH) Zürich, Switzerland. She is the Director of Georgia Tech's Center of Organic Electronics and Photonics, and was elected a 2023 Member of the European Academy of Sciences (EurASc); a 2021 Fellow of the U.S. National Academy of Inventors (NAI); a 2019 Fellow of the Materials Research Society (MRS); and a 2012 Fellow of the Royal Society of Chemistry (RSC). Her research interests encompass the broad area of functional polymer materials, polymer physics, organic electronics & photonics, and bioelectronics.



# Innovative Nanomanufacturing Paradigms for Sustainable Large-Area Electronics

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## Abstract

Adapting existing manufacturing methods to emerging forms of large-area nanostructured electronics presents major technological and economic challenges. Despite the difficulties, several new processing concepts have gained ground, transforming the broader marketplace and relevant manufacturing infrastructure. In this talk, I will discuss our recent efforts toward scalable manufacturing of emerging forms of large-area nanostructured electronics. I will show how developing innovative patterning technologies with engineered nanomaterials, can lead to more sustainable forms of optoelectronics with high-performance characteristics. Particular emphasis will be placed on the development and evolution of adhesion lithography (a-Lith) and self-forming nanogap lithography techniques and their use in an expanding range of applications, from ultra-fast optoelectronics to new chemical reactors and sensors.

**Short bio:**

Thomas D. Anthopoulos is a Material Science and Engineering Professor at King Abdullah University of Science and Technology (KAUST) in Saudi Arabia. He received his B.Eng. and D.Phil. degrees from Staffordshire University in the UK. He then spent two years at the University of St. Andrews (UK), where he worked on organic semiconductors for application in light-emitting diodes before joining Philips Research Laboratories in The Netherlands to focus on printable microelectronics. From 2006 to 2017, he held faculty positions at Imperial College London (UK), first as an EPSRC Advanced Fellow and later as a Reader and full Professor of Experimental Physics. His research interests are diverse and cover the development and application of novel processing paradigms and the physics, chemistry, and application of functional materials.



# Towards Robust Organic Solar Cells Based on Responsible Materials Printed from Water

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## Abstract

Printable organic photovoltaic solar cells (OPV), i.e. polymer solar cells, have now reached impressive power conversion efficiencies at lab scale over 19%. It is one crucial milestone towards the deployment of OPV products in real life. OPV holds many promises including potential low cost, large scale, low temperature processing, low energy payback time, low carbon footprint for the production of photovoltaic modules exempt of critical raw materials. However, today, not all are yet scientifically achieved. For example, commercially available OPV modules suffer from low PCE, from 3 to 5 % (30-50 Wp/m<sup>2</sup>) and are made with still costly raw materials mostly processed from toxic organic solvents. It is a matter of time for the industrial players to catch up with recent academic research to push industrial OPV performances further. This presentation will focus on three of our recent results: (1) a doping strategy to enable a homojunction hole extraction layer for improved efficiency and stability of OPV, (2) the processing of OPV active layer from water based inks as the ultimate non-toxic, responsible printing with record efficiencies thanks to nanoparticles control and surface energy matching, (3) the investigation on the impact of synthesis impurities, such as metal catalyst residues, on the performances of OPV to design a strategy for cost-effective purification of raw materials.



**Short Bio:**

Guillaume Wantz graduated from the School of Chemistry and Physics of Bordeaux (ENSCPB) in 2001 including a thesis work at Philips Research (Eindhoven, NL) on ink-jet printing. He received his Ph.D. in Electronics Engineering from the University of Bordeaux in 2004 working on Polymer Light Emitting Diodes. He was Assistant Professor at the University of Bordeaux working on Organic Field Effect Transistors with research stays at Queen's University (Kingston, Canada). In 2006, he was appointed as tenure Associate Professor at the Bordeaux Institute of Technology (Bordeaux INP). He is Professeur des Universités since 2021. His research interest is on Organic Electronics with a focus on polymer photovoltaic solar cells (OPV). He was invited-professor at Queen's University (Kingston, Ontario, Canada) in Spring 2012 and at Univ. of Massachusetts (Amherst, USA) in Fall 2014. He has been appointed at the "Institut Universitaire de France" (IUF Paris) in 2016. Since 2017, he is Associate Editor for the journal "Materials Chemistry Frontiers" (RSC). He is co-founder of Héole, a company developing flexible OPV products including solar-powered sails for yachting, a solar zeppelin and some BIPV flexible OPV products. To date, he has published 125 research papers in peer-reviewed international journals and issued 7 patents ( $h = 37$  – 6000 citations – source Google Scholar).

Guillaume Wantz  
Professeur des Universités  
Member of Institut Universitaire de France (IUF)  
Head of CNRS network on Organic and Hybrid Photovoltaic  
Associate Editor "Materials Chemistry Frontiers" (RSC)

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# Metal-Organic Chalcogenolates – An Emerging Family of Low-Dimensional Hybrid Semiconductors

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## Abstract

Metal-organic chalcogenolates (MOCs) are an emerging family of low-dimensional hybrid organic-inorganic semiconductors that combine the robustness of inorganic materials with the fabrication convenience and tunability of organic semiconductors. Silver phenylselenolate (AgSePh), a prototypical member of the MOC family, is a 2D semiconductor that features multiple exciting properties including narrow blue luminescence, in-plane anisotropy, large exciton binding energy, robust stability, non-toxic chemical composition, and scalable synthesis methods that are compatible with modern thin-film microelectronics manufacturing. Compared to other 2D semiconductors like layered perovskites and transition metal dichalcogenides, MOCs are distinguished by the presence of organic ligands covalently bound to their inorganic cores, which provides a unique handle to control their structures and electronic properties.

In this presentation, I will present advancement in the synthesis of MOCs, show the impacts of organic modification on their optoelectronic properties, provide examples of their applications in light emission and sensing, and discuss the insights into the exciton physics of this novel semiconductor family.

## Short Bio: Watcharaphol (Oat) Paritmongkol

### Professional Appointment

Lecturer, Vidyasirimedhi Institute of Science and Technology (VISTEC), Rayong, Thailand	2023-present
Research Focus: Hybrid Materials for Energy and Electronic Applications	

### Education and Training

Postdoctoral Fellow, University of Toronto, Toronto, Ontario, Canada	2021-2022
Advisor: Prof. Edward Sargent	
Project: Optoelectronic Applications of Nanomaterials	
PhD in Chemistry, Massachusetts Institute of Technology (MIT), Cambridge, MA, USA	2015-2021
Advisor: Prof. William A. Tisdale	GPA 5.0/5.0
Thesis: Syntheses and Photophysical Studies of Two-Dimensional Hybrid Organic-Inorganic Semiconductors	
Master of Chemistry, University of Oxford, Oxford, UK	2011-2015
(Awarded Jointly for Bachelor's and Master's education) First Class Honor	
Ranked 3 <sup>rd</sup> , 4 <sup>th</sup> , 9 <sup>th</sup> , and 5 <sup>th</sup> in 1 <sup>st</sup> , 2 <sup>nd</sup> , 3 <sup>rd</sup> , and 4 <sup>th</sup> years, respectively (class size ~180)	
Master Thesis Advisor: Prof. Philipp Kukura	
Thesis: Time-Domain Vibrational Spectroscopy with Compressed Probe Pulses	

### Awards & Honors

12. Best Poster Award, 2022 Materials Research Society (MRS) Fall Meeting 2022
11. Young Scientist Ambassador at the 71th Lindau Nobel Laureate Meeting 2022
10. Best Poster Award, 2021 Materials Research Society (MRS) Fall Meeting 2021
9. MIT Finalist to the Schmidt Science Fellow Program 2021
8. Young Scientist Ambassador at the 70th Lindau Nobel Laureate Meeting 2021
7. Best Poster Award, 2020 Materials Research Society (MRS) Fall Meeting 2020
6. Postmastership, University of Oxford 2013-2015
5. Fowler Prizes (x4), University of Oxford 2011-2014
4. Eisai Prize, University of Oxford 2013
3. Bruker Prize, University of Oxford 2012
2. Four Gold Medals and One Bronze Medal, the British Science Olympiads 2010-2011
1. DPST Scholarship, the Royal Thai Government 2009-2021

## Design of High Performing Conjugated Polymers with Low-Synthetic Complexity

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### Abstract

The performance of a range of organic electronic devices, from photovoltaics (OPV) cells to organic electrochemical transistors (OECTs) has made impressive progress over recent years, in part due to improvements in material design and synthesis. However, some of the resulting active materials now require complex, multi-step synthesis, potentially limiting their implementation at larger scale. Here I will discuss approaches to readily prepare building blocks in just one or two steps. Such approaches allow the preparation of conjugated polymers of low synthetic complexity which can be readily upscaled. I will highlight how this approach can be used to readily build libraries of conjugated polymers to more rapidly identify promising materials for application in OPV and OECT devices. Finally approaches to introduce additional functionality via post-polymerisation backbone modification will be discussed.

### **Short Bio: Prof. Martin Heeney**

Martin Heeney is a Professor of Chemical Science at King Abdullah University of Science and Technology (KAUST). He is a graduate of the University of East Anglia and received his PhD from the same institution in 1999 under the supervision of Prof. Michael Cook. Following a postdoctoral position with a start-up company in the area of photodynamic therapy, he joined Merck Chemicals in 2000, eventually becoming project leader for the organic electronics team. He made the move to academia in 2007, joining the Materials Department at Queen Mary University of London as a senior lecturer. In 2009 he moved across London to join the Chemistry Department at Imperial College London. His research interests include the design, synthesis and characterisation of conjugated materials for a variety of applications. He has published over 400 research papers, 5 book chapters and over 100 patents. His work has been cited over 34,000 times and he has an h-index of 97. He has been named five times by Thomson Reuters as a Highly Cited researcher in the field of Materials Science, is a recipient of the RSC Corday-Morgan (2013) medal, the RSC Peter Day (2020) award and the Macro group UK medal (2020).

### **EMPLOYMENT RECORD**

Imperial College London, Dept. Chemistry  
Professor of Organic Materials.  
Reader of Materials Chemistry  
Senior Lecturer May  
King Abdullah University of Science and Technology (KAUST), Saudi Arabia  
Professor of Chemistry, KAUST Solar Center  
Queen Mary University of London  
Senior lecturer in the School of Engineering and Materials.  
Flexink Ltd, Southampton  
Co-founder and director.  
Merck Chemicals Ltd, Southampton  
Project Leader, Organic Electronics Group  
Senior Scientist, Organic Electronics Group  
Research Scientist, Organic Electronics Group  
Scientist, Liquid Crystal Research  
Gentian AS, Norwich  
Industrial postdoctoral research assistant in photodynamic therapy

### **EDUCATION**

Ph. D. in Organic Chemistry, University of East Anglia, UK 1994-1999  
Thesis: "Synthesis and Characterisation of some highly functionalised phthalocyanine and naphthalocyanine transition metal derivatives" Supervisor: Prof. Michael J Cook. (Viva date June 1999)  
B. Sc. in Chemistry with First Class Honours. University of East Anglia, 1991-1994  
Including second full year spent at the University of Massachusetts, Amherst, USA.

### **AWARDS**

2020 RSC Macrogroup UK medal  
2020 RSC Peter Day award outstanding contributions to, and advancement of, the field of Materials Chemistry.  
2018 ISI HighlyCited™ 2015 (top 1% most cited scientist for period 2006-2016)  
2017 ISI HighlyCited™ 2015 (top 1% most cited scientist for period 2005-2015)  
2016 ISI HighlyCited™ 2015 (top 1% most cited scientist for period 2004-2014)  
2015 ISI HighlyCited™ 2015 (top 1% most cited scientist for period 2003-2013)  
2014 ISI HighlyCited™ 2014 (top 1% most cited scientist for period 2002-2012)  
2013 RSC Corday-Morgan Medal  
2007 Teamwork in Innovation - Highly Commended, Royal Society of Chemistry  
2007 Printed Electronics Best Technical Development – Materials, IDTechEx  
2006 Best Research and Development Achievement, Organic Semiconductor Industry Award  
2006 Organotechno Award, Japan 2006

# From UV to Near-Infrared light Detection: Next Generation Photodetectors for Imaging and Biometric Applications

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## Abstract

The current success of organic semiconductor technology is mainly driven by the development of organic light-emitting diodes (OLED), which are now routinely employed in display technologies. In the last decade, however, organic photovoltaics (OPV), leveraging the impressive improvement in device efficiency and stability, have gradually moved from a lab curiosity to a niche market. Their recent success has coincided with the rapid development of effective replacements for the fullerene-based materials that have been prevalent as electron acceptor materials until recently; namely the small molecule nonfullerene acceptors (NFAs). This relatively new class of materials offer a number of opportunities to develop new areas of research. Between those, organic photodetector (OPD), a technology based on organic photodiodes and thus closely related to OPV, is one of the most exciting. Recent efforts in the field of OPD have been focused on extending broadband detection into the near-infrared (NIR) region. The early absorption cut-off of solution processed organic semiconductors presents a challenge in achieving NIR detection, however, careful tuning of their chemical structures can help extend OPD responsivity into the infrared window. Here, we discuss how to design donor:acceptor blends and control charge carrier recombination in organic photodetectors for NIR light-to-current conversion for high efficiency and stable devices.

**Short bio:**

Dr. Nicola Gasparini received his B.Sc. and M.Sc, in Chemistry and Organic Chemistry, and Photochemistry and Molecular Materials, respectively, from the University of Bologna, Italy. In 2014 he joined the group of Professor Brabec in the Institute of Materials for Electronics and Energy Technology (i-MEET) at the Friedrich Alexander University Erlangen-Nürnberg (FAU) and received his PhD in 2017. In September 2017, he joined the King Abdullah University of Science and Technology (KAUST) as a postdoctoral fellow. In September 2019, he moved to the Department of Chemistry of Imperial College London as an independent researcher holding the Imperial College Research Fellowship. In early 2022, Nicola was appointed Lecturer in Chemistry (assistant professor, tenured) in the Department of Chemistry. He made major scientific contributions regarding the photophysical properties of organic semiconductors, resulting in over 100 publications. His research interests are in organic semiconductors, with particular interests in charge transport and recombination processes in organic solar cells and photodetectors.

## Thin Films for Multiplex Applications: Solar Cell, Light Emitting Diode, Photodetector, and Radiative Cooling Film

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### Abstract

Thin films are simple and innovative materials useful for countless applications due to minimal materials usage along with great practical impact. Perovskite thin films have gained tremendous attention for various applications in optoelectronics due to their charge/photon conversion capability and simple fabrication via solution processing i.e., spin coating, spray coating, dipping coating, and roll-to-roll printing. As precursor inks are in liquid form, doping and compositional tuning are facile. Due to the fact that precursor inks solidify into perovskite thin films, solvent engineering techniques, which affect perovskite nucleation and crystallization processes, along with perovskite compositions orchestrate both physical and chemical properties, leading to desired applications such as solar cell, light emitting diode, and photodetector. In the similar fashion, radiative cooling films can be fabricated via solution processing or polymer extrusion, which allows facile compositional and morphological tuning to maximize radiative release into the atmospheric transparency window. In this talk, we will discuss both thin film technologies investigated at our laboratory at Mahidol University.

*Keywords: Perovskite Solar Cell, Radiative Cooling Film, Perovskite Light Emitting Diode, Perovskite Photodetector, Thin Films for Energy Applications*

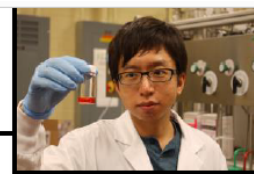




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### CONCENTRATIONS

Perovskite Solar Cells, Perovskite Light Emitting Diodes, Radiative Cooling Films, Condensed Matter Physics, Device Physics, Quantum Dot, Nanotechnology, Nanoscale Materials, Nano Sensors, Nanomechanics, Self-Assembly, Microscopies, Coating Technologies, and Lasers.

### BRIEF SUMMARY

Assoc. Prof. Dr. Pongsakorn received his B.A. in physics and economics from Washington University in Saint Louis in 2008. He earned his Ph.D. in physics from the University of Chicago in 2013. In collaboration with Argonne National Laboratory, Pongsakorn investigated self-assembly, nanomechanics, and application of solution-processed nanoparticle films. Because of his interests in both academic and business sides of R&D, he supplemented his business knowledge at the University of Chicago Booth School of Business. In 2013, Pongsakorn joined the Sargent lab at Electrical and Computer Engineering at the University of Toronto, one of the world-leading laboratories in colloidal quantum dot-based materials and perovskite and well known for the current world-record for CQD solar cells, as a postdoctoral fellow to work on solution-processed solar cells, light emitting diodes, lasing materials, and light detectors. Currently, Pongsakorn is the head of Advanced Technologies for Energy and Sustainability Lab at School of Materials Science and Innovation, Faculty of Science at Mahidol University in Thailand. His current research interests include solution-processed semiconductors i.e. perovskite solar cells and LEDs and radiative cooling films for heat reduction in building. He has published more than 70 international publications with more than 7000 citations and earned 2 Thai petty patents (5 more pending patent and 6 more pending petty patents). He always enjoys his time working with various undergraduate and graduate students in materials science with funding from both government agencies and industries, together exploring science and developing innovation.

### BACKGROUND



**Mahidol University**, faculty member at School of Materials Science and Innovation, Nakhon Pathom, Thailand *October 2015 - Now*

- Research Area: perovskite solar cells, light emitting diodes, radiative cooling films, nanomechanics and nanotechnology, solution-processed technologies, and physics of thin films.



**The University of Toronto**, Postdoc in Electrical and Computer Engineering, Toronto, ON

*September 2015*

- Research Area: nanotechnology, solar cells, and light emitting devices.
- Postdoctoral Advisor: Prof. Edward (Ted) H. Sargent, the Canada Research Chair in Nanotechnology.



**The University of Chicago**, Ph.D. in Physics, Chicago, IL

*August 2013*

- Ph.D. Advisor: Prof. Heinrich M. Jaeger, William J. Friedman and Alicia Townsend Professor of Physics.
- Ph.D. Committee: Prof. Thomas A. Witten and Prof. Dmitri Talapin.

**The University of Chicago**, M.S. in Physics, Chicago, IL

*August 2009*



**Washington University in Saint Louis**, B.A. in Physics and Economics, Saint Louis, MO

*May 2008*

- GPA: 3.97/4.00; Summa Cum Laude.
- Research Advisor: Prof. Stuart A. Solin. Research: Magnetic properties of S= 1/2 quasi-triangular lattice materials.

### EXPERIENCES

**School of Materials Science and Innovation, Faculty of Science, Mahidol University**

*October 2015 – Present*

Faculty member, Head of the “Advanced Technologies for Energy and Sustainability” Lab

- Colored perovskite solar cells for window replacement
- Perovskite solar cell for high humidity environment
- Solvent engineering techniques for low cost and high performance optoelectronics
- Perovskite LEDs and luminescent properties
- Radiative cooling films to reduce heat from buildings via low cost and scalable process.
- Materials science, nanotechnology, and nanoscale characterization
- Thin films, surfaces, and coating technologies
- Slot-die printing and flexible electronics

**Sargent Lab, University of Toronto**

*November 2013 – September 2015*

Postdoctoral Fellow

## What is special about Y6; the working mechanism of neat Y6 organic solar cells

Safa Shoaee<sup>a,\*</sup>

<sup>a</sup>*Optoelectronics of Disordered Semiconductors, University of Potsdam, Institute for Physics and Astronomy,  
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### Abstract

Exceptionally high quantum efficiencies with very small energy difference between the donor and the acceptor molecules have raised questions regarding the driving force for charge generation in organic solar cells. In light of this, we analyse the working mechanism of single component small molecule acceptor Y6 solar cells with power conversion efficiencies reaching up to 4.5% and short circuit currents up to 8.4 mAcm<sup>-2</sup>. Using Hall effect, photo-Hall, and photoinduced absorption (PIA) measurements, we show that the charge photo-generation occurs in the bulk of Y6. With the aid of space charge limited current (SCLC) measurements we show that Y6 has an ambipolar charge carrier mobility. Our data shows that the limiting factor for the power conversion efficiency is fast charge recombination, which can be suppressed in presence of the transport layers, or modifying the morphology with a solvent additive.

*Keywords: Y6, single component solar cell, charge generation*

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• **RESEARCH INTEREST**

My research is focused on understanding device physics and spintronics of next-generation semiconductors aiming for state-of-the-art green solar cells, light sensing applications, and notable over the horizon ideas such as the artificial retina and quantum computing. To this end, I use and develop steady state and time resolved spectroscopy techniques.

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• **CURRENT POSITION**

2023 – Joint professorship position at University of Potsdam and Paul Drude Institute, Germany.  
2018 – Associate Professor of Physics  
Institute of Physics and Astronomy, University of Potsdam, Germany.  
2016 – Group Leader; Sofja Kovalevskaja Laureate  
Institute of Physics and Astronomy, University of Potsdam, Germany.

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• **UNIVERSITY EDUCATION**

2010 Ph.D. (Physical Chemistry Awarded May 2010)  
Department of Chemistry, Imperial College London, U.K.  
PhD Supervisor: Prof James R. Durrant  
2006 MPhys. (Honours: BSc and MSc): Physics with Technological Physics  
Department of Physics and Astronomy, University of Manchester, U.K.

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• **SCIENTIFIC DEVELOPMENT**

2014 – 2016 Research Fellow Spectroscopist  
Centre for Plastic Electronics, The University of Queensland, Australia  
2013 – 2014 Senior Research Scientist  
National Physical Laboratory, U.K.  
2010 – 2013 Postdoctoral Research Associate  
Faculty of Natural Sciences, Imperial College London, U.K.  
2010 – 2012 Visiting researcher – several months in the two year period  
Georgia Institute of Technology, United States of America.

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# Engineering Performance and Stability Enhancements in Perovskite Photovoltaics

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J. D. Durrant<sup>b</sup>, M. Heeney<sup>b5</sup> and M. A. McLachlan<sup>a</sup>

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<sup>b</sup>Department of Chemistry, Molecular Sciences Research Hub, White City, London, W12 0BZ

<sup>1</sup>Now at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU); Helmholtz Institute Erlangen-Nürnberg

<sup>2</sup>Now at National Chung Hsing University, Taiwan

<sup>3</sup>Now at Eindhoven University of Technology

<sup>4</sup>Now at School of Engineering and Materials Science, Queen Mary University of London

<sup>5</sup>Now at King Abdullah University of Science and Technology (KAUST)

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## Abstract

Metal halide perovskites (MHPs) continue to stimulate interest, generate significant research volume, and fuel tremendous scientific discussion and debate. The rapid evolution and deployment of MHPs to the commercial realm has been a remarkable journey, and one which has occurred at unprecedented speed. These materials, and their precursors, afford numerous synthetic pathways from a plethora of starting materials via a variety of processes – the sum of which are complex, multi-component functional materials around which numerous scientific questions remain unanswered. Here we investigate the role of additives and post-deposition processing and their influence of morphology and microstructure on photovoltaic device performance and MHP stability.

Many strategies have emerged for tuning the properties of MHPs from substitutional doping to influence bandgap and electronic properties to additive incorporation to tune lifetime and stability – collectively resulting in a diverse range of compositions or “flavours” of MHPs being reported. Here I will discuss strategies reliant on additive incorporation that result in improvements in photovoltaic device performance and stability. In parallel we consider the interaction such additive molecules have with the MHP films and by utilising a range of correlative characterisation techniques we probe the location where our additives reside and the influence they have on the microstructure and morphology. By carrying out systematic studies of isolated MHP films, films sandwiched with interlayers and complete devices we explain the key relationships between structure, composition, and performance of our additive engineered perovskite solar cells.

**Keywords:** Perovskite, Photovoltaic, Additive Engineering, Processing, Materials Characterization

# Molecular Engineering of Hole Transporting Molecules for High Efficient and Enhanced Thermal Stability Perovskite Solar Cell

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Seul-Gi KIM<sup>b</sup>, Kai ZHU<sup>b</sup>, Nam-Gyu PARK<sup>c</sup>

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## Abstract

We report here the design and synthesis of different series of conjugated molecules for use as charge transporting materials in halide perovskite solar cells. The thermal, morphological, optical and electrochemical properties of all prepared compounds have been investigated in detail and a comparative discussion has been presented. Their characteristics have suggested that these molecules could be suitable for use as hole transporting materials in perovskite photovoltaic devices. The preliminary photovoltaic application have given devices with power conversion efficiency (PCE) around 17 %. Selected molecules have been subjected for further device optimization and in deep interface engineering (between the perovskite and hole transport layers) improving PCE to higher than 23 % and this champion PCE is even higher than that of the Spiro-OMeTAD-based device. Thermal stability test at 85 oC for over 1000 h showed that the PSC employed novel HTM retains 86% of initial PCE, while the Spiro-MeOTAD-based PSC degrades unrecoverably. Time-of-flight secondary ion mass spectrometry studies combined with Fourier transformed infrared spectroscopy reveal that novel HTM shows much lower lithium ion diffusivity than spiro-MeOTAD due to a strong complexation of the lithium ion with HTM, which is responsible for the higher degree of thermal stability. Under optimized condition, the perovskite solar cells employed additive-free HTM gave a PCE of ca. 16%. This work delivers an important message that capturing mobile Li<sup>+</sup> in hole transporting layer is critical in designing novel HTM for improving thermal stability of PSCs. In addition, it also highlights the importance of interfacial engineering on the non-conventional HTM.

## References:

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2. S.-G. Kim, T. H. Le, T. de Monfreid, F. Goubard, T.-T. Bui, N.-G. Park, *Advanced Materials* 2021, 33, 2007431. <https://doi.org/10.1002/adma.202007431>.

**Keywords:** *Perovskite Solar Cell, hole transporter materials, photovoltaic*

**Short Bio: Fabrice GOUBARD**

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**EDUCATION AND TRAINING**

M.Sc. in Engineering (Physical Chemistry) 1993	Sorbonne University	France
Doctor (Science of materials) (Distinction) 1996	Sorbonne University	France
Visiting researcher 1997	Hahn-Meitner-Institut	Germany
Ass. Professor 1996	CY Cergy Paris University	France
Habilitation (functional materials) 2007	CY Cergy Paris University	France
Full Professor 2008	CY Cergy Paris University	France

**RESEARCH ACTIVITIES**

Research activities of Fabrice Goubard are focused on the elaboration of functional hybrid nanomaterials for different applications. In photovoltaic domain, his study concerns mainly both stretchable solar cells and n-p interface between a mesoporous metal oxide and a conjugated polymer (or p-type molecule) in perovskite solar cells. Molecular engineering versus optoelectronic applications constitutes also one of his main subject. A non-negligible part of his research is also dedicated to heritage materials (identification and dating). He is currently the co-author of 123 publications, 1 patent and three book chapters and has given 12 invited lectures along with more than 35 oral and poster presentations in International Scientific Conferences. He is currently director of 2 on going doctoral thesis K Tambwee (in co-tutelle with UWC (South Africa) and E. André (with CSTB society). He is in close collaboration with Pr. N.G Park (Sungkyunkwan University, Korea) (STAR Project , Campus France) and Pr. J Jakmunee, N. Kungwan (Chiang Mai University, Thailand), Pr A. Amassian (NCSU, United States)

**5 MOST RELEVANT PUBLICATIONS (H-index: 34/ 123 publications)**

1. Nanographene Coupled with Interfacial Pyrene Derivatives for Thermally Stable Perovskite Solar Cells, S.G Kim, T. de Monfreid, J.H. Kim, F. Goubard, J.J. Berry, K. Zhu, T.T. Bui, N.G. Park. ACS ENERGY LETTERS, 8(5), doi:10.1021/acsenergylett.3c00262. 2023
2. Capturing Mobile Lithium Ions in a Molecular Hole Transporter Enhances the Thermal Stability of Perovskite Solar Cells, SG Kim, TH Le, T de Monfreid, F Goubard, TT Bui, NG Park, ADVANCED MATERIALS 33 (12), 2007431, 2021
3. Pushing the limits of flexibility and stretchability of solar cells: A review, E. Dauzon, X. Sallenave, C. Plesse, F. Goubard, A. Amassian, T. D Anthopoulos, ADVANCED MATERIALS, 33(36), 2101469, 2021
4. Stretchable and Transparent Conductive PEDOT:PSS-Based Electrodes for Organic Photovoltaics and Strain Sensors Applications. E. Dauzon, Y. Lin, H. Faber, E. Yengel, X. Sallenave, C. Plesse, F. Goubard,\* A. Amassian,\* and T.D. Anthopoulos, ADVANCED FUNCTIONAL MATERIALS, DOI: 10.1002/adfm.202001251, 2020
5. Conducting polymer nanostructures for photocatalysis under visible light Srabanti Ghosh S., Kouamé N. A., Ramos L., Remita S., Dazzi A., Deniset-Besseau A., Beaunier P., Goubard F., Aubert P-H. and Remita H. NATURE MATERIALS Volume: 14 , 5 , 505-511, 2015

# Advancements in 3D Integration: Challenges and Possibilities

Rino Choi<sup>a</sup>

<sup>a</sup>3D Convergence Center and Materials Science and Engineering at Inha University, Incheon 22212, Korea

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## Abstract

As electronic device dimensions shrink to a few tens of nanometers, the conventional path of 2-dimensional scaling appears to be reaching its inherent limitations. Rapid scaling down of devices in integrated circuits has historically led to enhanced integration density, improved device performance, and cost reduction. However, achieving further gains in areal integration density necessitates substantial investments in both time and resources. In parallel, modern system requirements demand more functionalities within confined spaces. Consequently, there has been a surge of interest in 3-dimensional stacking of device layers.

Unlike traditional 2D scaling, 3D integration offers a means to accommodate increasing demands within a smaller footprint. To supplant the conventional system-on-chip approach, successful 3D integration must exhibit a high density of interconnections. This presentation delves into the realm of high interconnect density technologies in 3D integration. The technique involves assembling integrated circuits by vertically stacking multiple device layers of high-quality crystalline semiconductors. Particularly, the focus lies on monolithic 3D (M3D) integration, a prominent method that involves forming multiple semiconducting device layers separated by interlayer dielectric (ILD) layers. A crucial consideration is conducting these stacked assemblies within a temperature range lower than approximately 450 °C to prevent thermal degradation of underlying device layers and interconnect metals.

Another technique in the realm of 3D integration is hybrid bonding, which employs a dielectric bond embedded with metal to establish interconnections. This approach allows for increased connectivity without the necessity of solder bumps on the devices. Nonetheless, the adoption of these technologies hinges upon the development of innovative process techniques and the resolution of various technical challenges.

The presentation provides an overview of the current state of 3D integration development while discussing the requisite technologies that need to be further developed to achieve successful implementation.

*Keywords: Integrated circuit, monolithic 3D, hybrid bonding*

## Facile Process to Control the Phase of Ferroelectric $\text{HfO}_2/\text{ZrO}_2$ Composite Dielectrics using CW Laser Annealing

Byoung Hun Lee<sup>a,\*</sup>

*<sup>a</sup>Center for Semiconductor Technology Convergence, Dept. of Electrical Engineering, Dept. of Semiconductor Engineering,  
Pohang University of Science and Technology,*

\*Corresponding Author's E-mail: bhlee1@postech.ac.kr

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### Abstract

Scaled semiconductor memory device requires capacitor dielectrics extremely scaled in terms of electrical thickness (higher dielectric constant) while keeping the leakage current to the minimum level (higher bandgap). Yet, the trade off between the band gap and the dielectric constant limits the further development of capacitor dielectric. Alternative approach is to create a highly polarizable dielectric while keeping the bandgap same by modulating the crystalline phase of high-k dielectric. Most efficient way to achieve the highest dielectric constant is to form a ferroelectric material having morphotropic phase boundary (MPB) structure. In this talk, we introduce a facile process to achieve MPB structure from the  $\text{HfO}_2/\text{ZrO}_2$  mixture using continuous wave (CW) laser annealing. A scaled semiconductor memory device necessitates capacitor dielectrics with highly scaled electrical thickness (increased dielectric constant), all the while minimizing leakage current (higher bandgap). Nevertheless, the trade-off between band gap and dielectric constant imposes constraints on the further advancement of capacitor dielectrics. An alternate approach involves producing a remarkably polarizable dielectric while maintaining the same bandgap, accomplished by manipulating the crystalline phase of the high-k dielectric. The most effective means of attaining the highest dielectric constant involves the creation of a ferroelectric material with a morphotropic phase boundary (MPB) structure. During this presentation, we present a straightforward method for achieving the MPB structure using continuous wave (CW) laser annealing in a  $\text{HfO}_2/\text{ZrO}_2$  mixture.

*Keywords: Ferroelectric, laser anneal, phase control, capacitor, dielectric constant*



# Magnetic Enantioseparation and Chirality-Induced Spin Selectivity

Hiroshi M. Yamamoto<sup>a,b\*</sup>

<sup>a</sup>*CIMoS/QuaRC Institute for Molecular Science, Myodaiji, Okazaki, Japan*

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## Abstract

The words true and false chirality have been coined by Barron in 1980's in order to discuss chirality of objects including their motions [1]. In his discussion, the original chirality defined by Lord Kelvin should be defined as parity(*P*)-odd and time-reversal(*T*)-even pseudo scalar while a “false” chirality can also emerge in *P*-odd *T*-odd systems. In this regard, so called “chiral superconductor” where *T* symmetry is broken is a falsely chiral system, or even is not at all chiral in terms of *P* symmetry. In any case, symmetry consideration both in *P* and *T* symmetries is essential in understanding quantum system with asymmetric structures.

Chirality-Induced Spin Selectivity (CISS) is attracting recent attention as a new source of spin polarized current. It also provides unique methods for enantio-separation [2], enantio-selective electrochemical reactions, and an efficient water oxidation. The mechanism of CISS effect is, however, yet to be clarified, as the effect is much larger than expected one estimated with small spin-orbit coupling for organic molecules. In a hypothetical consideration, it is proposed that an enhancement of spin polarization is associated with anti-parallel spin polarizations at two opposite ends of a chiral molecule. It is interesting to note that such an anti-parallel spin pair is *T*-odd state, while the chiral molecular structure is *T*-even. We think symmetry conversion from *T*-even to *T*-odd quantities gives an essential clue to understand CISS effect that can generate huge spin polarization in a non-equilibrium condition.

We have made such a symmetry consideration based on multipole basis and found that a *T*-odd chirality can emerge from an accumulation of *T*-even spin current (= electrical toroidal monopole) at reservoirs [3]. Experimentally, we have shown that chiral organic superconductor can exhibit spin accumulation at two opposite crystal edges whose directions are anti-parallel to one another [4]. This can be regarded as a macroscopic-size emulation of chiral molecules that has *T*-odd spin accumulations at their opposite ends. Enantio-separation of helical noncovalent nanowires by magnetic substrates will be also discussed [5].

## References

- [1] L. D. Barron *Chem. Soc. Rev.* **15**, 189 (1986)
- [2] K. Banerjee-Ghosh *et al.*, *Science* **360**, 1331 (2018)
- [3] J. Kishine, H. Kusunose, and HMY, *Isr. J. Chem.* **62**, e202200049 (2022)
- [4] R. Nakajima, HMY *et al.*, *Nature* **613**, 479 (2023)
- [5] H. Aizawa, HMY *et al.*, *Nature Commun.* **14**, 4530 (2023)

**Keywords:** Chirality, Enantioseparation, Superconductivity, CISS, time-reversal symmetry

**Short Bio: Prof. Dr. Hiroshi Yamamoto**

Institute for Molecular Science

Hiroshi Yamamoto received his D. Sc. degree in solid state chemistry at University of Tokyo in 1998. After one year service as an assistant professor at Department of Physics, Gakushuin University, he spent 13 years as a research scientist at RIKEN. Since 2012, he serves as a full professor at Institute for Molecular Science, National Institutes of Natural Sciences in Japan. His research interests focus on organic electronics and spintronics based on novel operation mechanism. More specifically, an organic superconductor transistor and spintronic devices based on chirality are two major current topics in his study.

# Advancements in 3D Integration: Challenges and Possibilities

Rino Choi<sup>a</sup>

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## Abstract

As electronic device dimensions shrink to a few tens of nanometers, the conventional path of 2-dimensional scaling appears to be reaching its inherent limitations. Rapid scaling down of devices in integrated circuits has historically led to enhanced integration density, improved device performance, and cost reduction. However, achieving further gains in areal integration density necessitates substantial investments in both time and resources. In parallel, modern system requirements demand more functionalities within confined spaces. Consequently, there has been a surge of interest in 3-dimensional stacking of device layers.

Unlike traditional 2D scaling, 3D integration offers a means to accommodate increasing demands within a smaller footprint. To supplant the conventional system-on-chip approach, successful 3D integration must exhibit a high density of interconnections. This presentation delves into the realm of high interconnect density technologies in 3D integration. The technique involves assembling integrated circuits by vertically stacking multiple device layers of high-quality crystalline semiconductors. Particularly, the focus lies on monolithic 3D (M3D) integration, a prominent method that involves forming multiple semiconducting device layers separated by interlayer dielectric (ILD) layers. A crucial consideration is conducting these stacked assemblies within a temperature range lower than approximately 450 °C to prevent thermal degradation of underlying device layers and interconnect metals.

Another technique in the realm of 3D integration is hybrid bonding, which employs a dielectric bond embedded with metal to establish interconnections. This approach allows for increased connectivity without the necessity of solder bumps on the devices. Nonetheless, the adoption of these technologies hinges upon the development of innovative process techniques and the resolution of various technical challenges.

The presentation provides an overview of the current state of 3D integration development while discussing the requisite technologies that need to be further developed to achieve successful implementation.

*Keywords: Integrated circuit, monolithic 3D, hybrid bonding*

# Nanofabrication of Plasmonic Au-Nanohole Arrays via Direct- Impressing Process

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## Abstract

This study describes an efficient nanofabrication process of plasmonic metallic nanostructure on a substrate. Firstly, a silicon master mold of nanohole patterns with a diameter of 1,000 nm is prepared using photolithography. The hot stamping process was used to transfer the nanopattern from a master mold to a polymer film, Biaxially oriented polypropylene (BOPP), 100  $\mu\text{m}$  of thickness. On a film mold, nanopillar arrays with a diameter of 1000 nm were fabricated. Secondly, quartz substrate was cleaned for 15 minutes in an acetone bath. The sputter coating machine then coated a substrate with a thin gold film for a thickness of 30 nm. The sputter gas was Argon at about 15 Pa, a voltage of 0.8 kV, and a current of 10 mA. The coating time was adjusted to control the thickness of thin gold film. Finally, a BOPP film mold with nanopillar arrays was patterned onto thin gold film using direct-impressing technique. Tweezers were used to scrape the back side of the polymer film mold to add an impressive force. The protuberance of gold nanohole was examined using an AFM. It was confirmed that gold nanohole arrays with an average diameter of 1,000 nm were then constructed onto thin gold film. Furthermore, the optical properties of gold nanohole arrays were investigated. In an absorbance configuration, the ultraviolet-visible extinction spectra were measured using a light source with a spectrometer. The absorbance spectra are recorded in the visible light range. It was found that an absorbance peak appeared on the wavelength of about 550 nm. It was also confirmed that a regularity of nanohole structure arrays leads to higher and steeper enhancement of absorbance spectrum compared with the bare gold thin film on a substrate. These enhanced absorbance spectra could be tuned by the protuberance of gold nanostructure film on a substrate.

*Keywords: Direct impressing process, Gold nanohole arrays, Plasmonic metallic nanostructure, Absorbance spectrum, Polymer film mold*

# Deep Blue Emitter with a Combination of Hybridized Local and Charge Transfer Excited State and Aggregation-Induced Emission Features for Efficient Non-Doped OLEDs

Teerapat Itsoponpan<sup>a,\*</sup>, Praweena Wongkaew<sup>a</sup>, Taweesak Sudyodsuk<sup>b</sup>,  
Vinich Promarak<sup>a</sup>

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## Abstract

In this work, a deep blue solid state emitter, namely PI-TPB-CN, with a synergistic effect of hybridized local and charge transfer excited state (HLCT) and aggregation-induced emission (AIE) features is successfully designed and synthesized to improve the performance of deep blue organic light-emitting diodes (OLEDs). PI-TPB-CN is constructed using a 1,2,4,5-tetraphenylbenzene (TPB) as a  $\pi$ -conjugated AIE core being asymmetrically functionalized with a phenanthro[9,10-d]imidazole (PI) as a weak donor (D) and a benzonitrile (CN) as an acceptor (A), thereby formulating D- $\pi$ -A type fluorophore. Its HLCT and AIE properties are verified by theoretical calculations, solvatochromic effects, and transient photoluminescence decay experiments. The results reveal the existence of the reverse intersystem crossing between the high-lying triplet state ( $T_2$ ) and the lowest excited singlet state ( $S_1$ ), ensuring a strong blue emission (452 nm) with a high photoluminescence quantum yield of 74% in the thin film. PI-TPB-CN is successfully employed as a blue emitter in OLEDs. As a non-doped emitter, the OLED with the structure of ITO/HATCN (6 nm)/NPB (30 nm)/TCTA (10 nm)/PI-TPB-CN (30 nm)/TPBi (40 nm)/LiF (1 nm)/Al (100 nm) demonstrates excellent electroluminescence (EL) performance with blue emission ( $\lambda_{EL}$  = 451 nm) and maximum external quantum efficiency ( $EQE_{max}$ ) of 7.3%. The non-doped device with a thinner layer of PI-TPB-CN (20 nm) and TPBi (30 nm) layers exhibits a deeper blue emission ( $\lambda_{EL}$  = 444 nm) with CIE coordinates of (0.16, 0.09), a low turn-on voltage of 3.0 V, and  $EQE_{max}$  of 6.3%.

**Keywords:** Tetraphenylbenzene, deep-blue emitters, hybridized local and charge-transfer (HLCT), aggregation-induced emission (AIE), organic light-emitting diode

## A Switchable Ionic Diode Membrane Enabled by Covalent Organic Framework and PET Conical Nanochannels

Chia-An Lung <sup>a</sup>, Ting-Yi Huang <sup>a</sup>, Yu-Chun Su <sup>a</sup>, Li-Hsien Yeh <sup>a\*</sup>

<sup>a</sup>Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei 10607, Taiwan.,

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### Abstract

Various efforts have been made to mimic the regulatory properties of the biological nanochannels that exist in cell membranes of certain living organisms. Such ion channels are able to generate electricity in response to changes in surrounding chemical potential (i.e., ion concentration gradient). In this work, we report the design and fabrication of an asymmetric ionic diode membrane (IDM) composed of a top layer of sub-3 nm-scale covalent organic framework (COF) channels and a bottom layer of polyethylene terephthalate (PET) conical nanopores. The designed IDM was found to exhibit ionic current rectification (ICR) over a wide range of electrolyte concentrations (1, 10, 100, 500 and 1000 mM) attributable to its structural asymmetry. Interestingly, we also observed an inversion of the ICR (i.e., from backward ICR to forward ICR) when pH was reduced from 6 to 3. Such pH induced ICR enhancement was found to be exceptionally stable as evidenced by the steady current values over 7 on/off cycles at both low (10 mM) and high (100 mM) electrolyte concentrations. A mechanism for the ion transport was proposed to explain the inversion phenomenon. This work highlights the pH-switchable ionic transport properties of the sub-3 nm-scale COF-based IDM, as well as its potential for long-term operation under high salinity conditions.

*Keywords: Nanofluidic Diode, Ion transport, Ion current rectification, Asymmetric nanochannel membrane,*

## Synthesis of Fe<sub>3</sub>O<sub>4</sub> Ceramic Magnet via Cold Sintering Process

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### Abstract

Cold sintering process (CSP) was utilized to prepare ceramic magnets made of magnetite (Fe<sub>3</sub>O<sub>4</sub>). This innovative method employs a low-temperature approach to overcome the phase-change challenges commonly encountered when synthesizing bulk Fe<sub>3</sub>O<sub>4</sub> ceramics. The liquid medium used in the process consisted of oxalic acid (OA) solution with varying concentrations (0 M, 0.05 M, 0.3 M, 0.55 M, 0.8 M, and 1.05 M). X-ray diffraction (XRD) analysis verified the successful synthesis of all samples as a cubic phase of magnetite. Notably, the use of oxalic acid as a solvent resulted in an enhanced microstructure and relative density compared to samples prepared with water. This improvement can be attributed to the partial dissolution of Fe<sub>3</sub>O<sub>4</sub> particle edge due to oxalic acid. Microstructural analysis using a scanning electron microscope (SEM) revealed the formation of "necks" between Fe<sub>3</sub>O<sub>4</sub> particles in the CSP-treated samples, which contributed to an increased density and denser microstructure. The enhanced microstructure positively affected the mechanical properties, as confirmed by Vickers hardness testing. Magnetic properties of the bulk ceramic magnets, investigated using a vibrating sample magnetometer (VSM), indicated typical ferrimagnetic behavior with a saturation magnetization ranging from 55.6 to 71.2 emu/g. These findings provide compelling evidence that the cold sintering process is a viable method for producing bulk Fe<sub>3</sub>O<sub>4</sub> ceramics without undergoing phase transformations.

*Keywords: iron oxide, cold sintering, magnetic, ceramic magnet.*

# Towards Perovskite-Based Next-Generation Electronics: n-Type Doping of Methylammonium Lead Iodide Thin Films

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## Abstract

Metal halide perovskites are known to be excellent candidates for semiconductors of the next-generation electronics. At the moment, to reach their full potential, the proper understanding and efficient control of doping is necessary. While doping is often confused with additives or interface engineering, we show a truly electronic doping, that leads to the increase of the electron density, resulting in the conductivity increase by 3 orders of magnitude. We present the substitution of the  $\text{Pb}^{2+}$  ions in the perovskite polycrystalline film by samarium metastable  $2+$  ions ( $\text{Sm}^{2+}$ ), which oxidize to  $\text{Sm}^{3+}$  once introduced into the lattice. Each of the oxidized samarium ion releases an electron to the conduction band of the semiconductor. The resulting perovskite is therefore n-type, which is confirmed by ultraviolet photoelectron spectroscopy (UPS), showing the shift of the Fermi level ( $E_F$ ) by 0.5 eV towards the conduction energy ( $E_C$ ) upon doping. The oxidation of samarium ions is confirmed by the Sm 3d core level in the X-ray photoelectron spectrum (XPS) analysis. The ionized charge carrier density is estimated from the Mott-Schottky plot to be  $10^{17} \text{ cm}^{-3}$  for the sample showing the highest conductivity increase, which corresponds to effective 0.1% doping concentration (Pb density in  $\text{MAPbI}_3 \approx 20^{21} \text{ cm}^{-3}$ ). The discrepancy between this result and the doping concentration stemming from the XPS measurement, which is calculated to be around 20%, leads to investigate the dopant activation energy that can be calculated from the Arrhenius plot of the conductivity vs. temperature. The dopant activation energy of around 350 meV is in correspondence with the energy between the  $E_F$  and  $E_C$ , i.e. the energy necessary to ionize all the dopants. This raises the possibility of the dopant freeze-out effect at room temperature, which could be responsible for only partial dopant activation in normal conditions.

*Keywords: metal halide perovskite, doping, next-generation electronics*



## Exploring Compositional Landscape of Triple Cation Perovskite to Achieve Functional Perovskite Solar Cell for Indoor Application

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### Abstract

Perovskite solar cell is a promising energy source for small electronics used in internet of things (IoT) due to its high absorption coefficient under low light condition and tunable bandgap. To achieve high performance under low light, proper bandgap close to 1.8 eV and low trap density are critical. This work adjusted the chemical composition of triple cation perovskite and identify its effects on physical and optoelectronic properties, including surface morphology, crystallinity, UV-Vis absorption, photoluminescence, time-resolved photoluminescence, external quantum efficiency, power conversion efficiency (PCE), and stability. Compositional landscape was explored, considering the variation of cations via Cs and of anions via mixed halides. Combining optimal composition with low-cost carbon-based electrode results in the highest PCE beyond 30% under 1000 lux indoor light with both phase and operational stability. Furthermore, the work sheds insights on hysteresis and trap density due to compositional effects, laying groundwork for future development of low light photovoltaics. Lastly, two 1-cm<sup>2</sup> solar cells developed in this work were connected in series to power multiple sensors at the same time to demonstrate its functionality under indoor light condition.

**Keywords:** Indoor Perovskite Solar Cell, composition tuning, carbon-based electrode, hysteresis, phase and operational stability

# High-Performance Perovskite/Organic Tandem Solar Cells

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## Abstract

The tunable bandgap of metal halide perovskite semiconductors makes them attractive for application as absorbers in multi-junction solar cells offering performance that surpasses that of conventional single-junction cells by utilizing a wider part of the solar spectrum [1, 2]. However, developing different perovskites with fully complementary absorption characteristics and similar performance remains challenging. One possible solution is to combine perovskite and organic sub-cells with complementary absorption characteristics. For example, combining a wide-bandgap (~1.80 eV) perovskite sub-cell with a narrow-bandgap (~1.33 eV) organic subcell yields perovskite/organic tandem cells with a significantly broader absorption spectrum and photovoltaic performance [3]. In such a configuration, the perovskite subcell harvests the blue part of the solar spectrum while letting red and near-infrared light pass through to be absorbed in the narrow bandgap organic subcell. In such devices, developing and using highly transparent charge transport layers and recombination junctions is critical for minimizing parasitic absorption and maximizing the power conversion efficiencies of the tandem solar cells. Recently, surface modification of transparent conductive electrodes, such as indium tin oxide and indium zinc oxide, with self-assembled organic monolayers has emerged as a new method for fabricating highly transparent charge-selective contacts [4]. Herein, we discuss the design and development of high-performance perovskite and organic subcells using self-assembled monolayer-modified interlayers and their deployment in high-efficiency hybrid tandem solar cells. Specifically, we will show how combining suitable metal oxides with surface-modifying agents enables the monolithic integration of the perovskite and organic subcells into tandem solar cells with record performance. Finally, we will highlight the developments required to push the performance of hybrid perovskite/organic tandem solar cells to levels well beyond that of single-junction devices.

**Keywords:** Perovskite solar cells, Organic solar cells, Tandem solar cells, Semiconductors, Interface engineering.

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## Energy-efficient Perovskite Solar Cell Production via Microwave Annealing Process and Carbon-based Additives

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### Abstract

Perovskite solar cell (PSC) is a promising photovoltaic technology to replace or supplement conventional solar cell technologies. The fabrication of high-quality perovskite solar cells via one-step spin coating with a sequential anti-solvent dropping method and thermal annealing is reported as an effective method to form perovskite crystals from solution-based precursors. [1] However, the traditional hotplate annealing is facing a challenge in terms of gradient heat transfer, resulting in non-uniform grain size and miscellaneous phase in perovskite surface structure. [2] Various works have studied the short exposure annealing with highly intense radiation to control the crystallization of perovskite crystal and reach fast and high-volume production. [3] Due to its quick, rapid, and energy-saving process, microwave heating is demonstrated as an alternative annealing process, converting electromagnetic energy to thermal energy directly. In this work, PSC via microwave annealing process has been investigated. With the incorporation of microwave-absorbing nanomaterials, crystallization and nucleation growth of perovskite crystal is induced and promoted. The experimental results indicate smooth and uniform surface along with lower trap density from a total irradiation time of less than three minutes. This process leads to planar indoor perovskite solar cells with efficiencies exceeding 20% at 1000 lux.

*Keywords: perovskite solar cell, microwave annealing process, electromagnetic radiation, carbon nanomaterial*

# Thermal Stability of Total Absorptivity in Metallic Oxide Nanotextured Surfaces for Enhanced Performance Selective Solar Coatings

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## Abstract

Selective solar coatings (SSCs) are crucial optical components capable of efficiently converting solar energy into thermal energy within concentrated solar-thermal energy systems operating under high temperatures. Metallic surfaces featuring nanotextured structures closely mimic the optical and thermal properties of an ideal SSC. This investigation focuses on the successful fabrication of a metallic oxide nanotextured surface on the surface of halide stainless steel 304 using the sparking process in ambient air conditions. Atomic force microscopy reveals the presence of distinct nanotextures on the fabricated sample's surface. Through Raman spectroscopy, the atomic vibrations of these nanotextured surfaces unveil the formation of iron and oxides. By employing UV-VIS-NIR spectroscopy with an integrating sphere, the total absorptivity of the nanotextured surface is measured. Additionally, the investigation delves into the thermal stability of the nanotextured surface by analyzing its total absorptivity following exposure to elevated temperatures. Overall, this study introduces a straightforward, cost-effective, and non-physical approach for producing high-performance SSCs. By showcasing the fabrication process and characterizing the resulting properties, our work contributes to the advancement of efficient and accessible solar energy conversion technologies.

*Keywords: selective solar coating, nanotexture, sparking process*

# Synthesis of Natural Rubber-Titanium Dioxide/Silver Nanocomposite for the fabrication of high performance Triboelectric Nanogenerator

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## Abstract

The rapid developments of the Internet of Things (IoTs) and artificial intelligence (AI) have essentially required an increasing demand for energy leading to the energy crisis. In addition, the use of fossil fuel also causes pollution problems affecting humans and the environment. Therefore, the development of clean and sustainable renewable energy technologies is important and is gaining a lot of attention. Here, we have fabricated a triboelectric nanogenerator (TENG), which is a new technology on energy harvesting that convert mechanical energy into electricity. The natural rubber nanocomposite with TiO<sub>2</sub>/Ag hybrid nanoparticles is synthesized and used as a triboelectric material for TENG. It is found that the synthesized hybrid nanoparticles can increase the TENG output power up to 13 folds higher than that of the unmodified NR TENG. This is attributed to the remarkable electrical properties of the nanohybrid materials. Moreover, the TENG prototype fabricated from the natural rubber nanocomposite is demonstrated to harvesting natural wind energy, which can generate electricity to light up LEDs. The findings of our work has proposed the new direction on the development of energy harvesting technology from natural materials toward with highvalue added products in the future.

*Keywords: Triboelectric nanogenerator, nanohybrid material, titanium dioxide nanoparticles, silver nanoparticles, natural rubber*

# Synthesis and Characterization of Diamond-Like Carbon Films with Different Proton Acceptor Hydrocarbon Electrolytes of Electrodeposition for Motion Sensor

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## Abstract

Diamond-Like Carbon (DLC) dielectric film has the outstanding hardness, frictionless, and adjustable electronic properties. It is used as both protective layer of mechanical part and insulated layer in electronic device. Its properties are controlled by its structure and chemistry which depend on synthesis method. Typically, DLC coating is carried out by a chemical vapor deposition (CVD) or physical vapor deposition (PVD) process that requires relatively sophisticated experimental set up under vacuum condition. Alternatively, DLC can be fabricated by an electrodeposition (ED) method which has lower cost than CVD process. ED process requires an organic carbon precursor into solution and a power supply to control the deposition condition under ambient atmosphere without the use of vacuum condition. Furthermore, ED technique allows the controls over surface morphology and film properties by deposited parameters. In this research, DLC film is fabricated and coated on stainless steel substrate using ED method with different proton acceptor electrolytes which are dimethyl sulfoxide, acetone, acetylacetone, and glycerol. The effect of carbon precursor type on DLC coating, film morphology, chemical structure, and electronic properties are studied and the correlation of the synthesis condition are discussed. This work has proposed the effective technique to fabricate DLC film under atmospheric pressure and room temperature which is green and cost-effective method that may be beneficial for the further development of electrode for motion sensing device.

*Keywords: Diamond-Like Carbon, Electrodeposition, Hydrocarbon Proton acceptor*

# Synthesis of cellulose paper from sugarcane leaves filled with magnetite nanoparticles for triboelectric nanogenerator application to harvest mechanical energy

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## Abstract

In this research, the cellulose paper is synthesized from sugarcane leaves and used to fabricate an energy harvesting device called a triboelectric nanogenerator (TENG) that convert mechanical energy into electricity based on contact electrification and electrostatic induction effects. The cellulose fibers are synthesized and modified by adding magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles which are prepared by co-precipitation technique in order improve the charge capacitance of the cellulose paper. The effect of  $\text{Fe}_3\text{O}_4$  nanoparticle loading on the energy production performance of the fabricated cellulose paper TENG is investigated. It is found that  $\text{Fe}_3\text{O}_4$  nanoparticles can promote triboelectric charge capacitance of the cellulose paper composite, which resulting in the enhancement of the TENG electrical output. The highest delivered electrical power of  $1.9 \text{ W/m}^2$  is obtained from the cellulose-  $\text{Fe}_3\text{O}_4$  paper TENG, which is double of the pristine cellulose paper TENG. The electrical power can charge a capacitor which is then used as a power source for a small and portable electronic device. This work has proposed the use of sugarcane leave which is one of the main agricultural wastes to develop a clean and sustainable power source.

*Keywords: cellulose paper, triboelectric nanogenerator,  $\text{Fe}_3\text{O}_4$ , sugarcane leaves*

## Performance of Carbon Nanotube Thermal Paste in Peltier Cooling Applications

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### Abstract

In recent years, there has been significant advancement in the development of semiconductor based thermoelectric Peltier modules due to its favourable integration into compact devices for commercial applications where less maintenance is needed, energy-saving properties and high precision temperature control compared to the conventional compressor technology. Potential electronic applications where Peltier modules will be advantageous includes portable coolers, water purifiers and electronic cooling electronic components and systems. The Peltier effect is a phenomenon in which the electric current passes through the junction connecting two materials in which one side becomes cold as electrical current passes through it, while the other side releases the heat extracted from the cold side into the environment. One of the crucial components to enhance the performance of Peltier effect is to be able to spread the heat quickly, hence a highly thermal conductive paste plays an important role to ensure improved efficiency. In this paper, we demonstrate the performance improvement of cold-water Peltier module by integrating carbon nanotube (CNT) thermal conductive paste as a heat spreader. The CNT thermal paste was applied to the Peltier module to enhance the heat transfer between the respective thermal interface. The thermal conductivity of the developed CNT thermal paste has an improved performance of 32.67% compared to the reference silver conductive paste and when integrated with Peltier cold water module, temperature of 9-12 °C was achieved with a water flow rate of 400-500 ml per minute as part of an IoT smart water purifier and dispenser system. As the system does not require the use of a compressor for cooling, significant energy savings up to 70% can be achieved.

*Keywords: carbon nanotube, thermal paste, peltier, thermal conductivity, cold-water module*



## Hot-Electron SERS Substrate for Solar Thermal coating

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### Abstract

Hot electron transfer between electrode surface and the adsorbate is a determining mechanism in numerous electrochemical technologies, for which the estimation of parameters controlling the charge transfer is important to electrode design and utilization. Herein, nanothin-Au/SiO<sub>2</sub>/Si electrodes are fabricated and analyzed for source, generation, energetic characteristic, and interfacial transfer process of photo-generated surface hot electrons in order to develop a charge-transfer (CT) surface-enhanced Raman scattering (SERS) platform for carbon nanocomposite inspection. To ensure high-quality Au nanofilm, sputtering coating technique is used with minimal chemical treatment of SiO<sub>2</sub>/Si surface. Considering nanoscale localized conductivity and workfunction of electrode surface acquired using atomic force microscopy with varying Au film thickness, strong contribution to SERS signal generation from free electrons of Si extracted toward Au surface is anticipated. Interpreting wavelength-dependent Raman spectroscopic data with varying Si doping concentrations together with calculated density-of-state distribution of methylene blue/Au interface, the obtained SERS performance is ascribed to CT mechanism induced by the indirect and the resonant surface plasmon-enhanced direct interfacial transfers of hot electrons originating from Si and from Au when excited by green and red lasers respectively. Applying the electrodes as a CT SERS platform to inspect a reduced graphene oxide/silica (rGO/SiO<sub>2</sub>) nanocomposite used for solar thermal coating, conducting-rGO-core/insulating-SiO<sub>2</sub>-shell structure which implies plasmonic-heating property is proposed and correlated with its light-to-heat conversion efficiency. In addition to that the findings on the hot-electron injector electrode shed light on its applicability and improvement for electrochemical technologies, those findings about the coating nanocomposite suggest efficiency enhancement based on plasmonic heating and the search for electron-rich additives complying to the circular green economy.

*Keywords: hot electron transfer, electrochemical electrode, plasmonic heating, solar thermal coating, nanomaterial*

# Effect of sintering temperature on the thermoelectric properties of Ag<sub>2</sub>Se fabricated by spark plasma sintering with high compression

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## Abstract

At near room temperature, Ag<sub>2</sub>Se is an attractive candidate to replace traditional high-performance thermoelectric (TE) materials, such as Bi<sub>2</sub>Te<sub>3</sub>. By varying the sintering temperature from 423 K to 723 K in the spark plasma sintering (SPS) process, along with using high compression of up to 300 MPa, it improves its TE figure-of-merit (ZT). The Ag<sub>2</sub>Se nanoparticles prepared by the wet chemical method were compacted using the high compression of SPS, leading to the rapid fusion of particles. This contributes to the creation of nanopores at the grain boundaries and cracks at high sintering temperatures. The size and number of pores increase with an increase in sintering temperature. These features decrease the carrier concentration, which significantly affects the TE properties. The electrical conductivity decreases from  $2.5 \times 10^5$  S/m to  $1.0 \times 10^5$  S/m at room temperature, while the absolute Seebeck coefficient increases from -100  $\mu$ V/K to -150  $\mu$ V/K at room temperature with an increase in sintering temperature. The activation energy ( $E_a$ ) tends to increase with an increase in sintering temperature, confirming that carrier transport is hindered by the porous structure. The decrease in carrier concentration also significantly suppresses electronic thermal conductivity, and the porous structure contributes to increased phonon scattering, resulting in a reduction of lattice thermal conductivity. The total thermal conductivity decreases from 1.5 W/mK to 0.8 W/mK. The high average ZT of 0.90 was observed in the bulk sample sintered at 723 K. Thus, high compression and sintering temperature are likely to be key factors in fabricating bulk Ag<sub>2</sub>Se with high TE performance.

*Keywords: Thermoelectric, Ag<sub>2</sub>Se, Spark plasma sintering.*

## Effects of Capping Agent on Tin Dioxide Nanoparticles Synthesized by Simple Precipitation Method

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### Abstract

In this work, nanoparticles of tin dioxide ( $\text{SnO}_2$ ) were synthesized by a simple precipitation method. Tin (II) chloride dihydrate ( $\text{SnCl}_2 \cdot \text{H}_2\text{O}$ ) and Sodium hydroxide ( $\text{NaOH}$ ) were used as starting material. Lemon-lime vitamin C water was used as a capping agent. The effect of the capping agent on the properties of  $\text{SnO}_2$  such as crystal structure, and morphology is investigated. The structural properties of the obtained samples were studied by X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscope (TEM). The chemical composition is analyzed by energy dispersive spectroscopy (EDS). Fourier Transform Infrared spectroscopy (FTIR) was used to determine the functional groups present in the sample. The XRD results showed that all  $\text{SnO}_2$  nanoparticle samples are in a tetragonal structure (JCPDS card, No.41-1445). There is a significant on the crystal size of the  $\text{SnO}_2$  nanoparticles with different capping agents. The smallest diameter of the nanoparticle can be obtained at about 11 nm via lemon-lime vitamin C water (10% of solution volume) while the obtained sample without capping agent shows a crystal size of about 60 nm. This indicated that the crystalline size of  $\text{SnO}_2$  nanoparticle decreased with capping agents. The SEM images showed all samples consisted of agglomerated spherical grains. The prepared samples had the expected elements, tin, and oxygen confirmed by the EDX analysis. Due to the small particle size and large surface area in contact, it can be used as a gas detector.

*Keywords:  $\text{SnO}_2$ , Nanoparticles, Tin dioxide, Precipitation method, Capping agent*

# Electrically Conducting PDMS Elastomer for Fluid Flow Detection

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## Abstract

Electrically conducting and flexible materials have received tremendous interest recently in many areas, such as sensors, intelligent robots, lightweight mobile electronics, biomedical applications, and wearable devices, as they can provide new device functionalities and reduce application complexities. Polydimethylsiloxane (PDMS) is a biocompatible and flexible material suitable for such flexible applications. However, PDMS is electrically insulating in nature limiting its applications in flexible electronics. Here, we report the development of an electrically conducting PDMS elastomer by incorporating multiwalled carbon nanotubes (MWCNTs) into the PDMS matrix, where silane-modified cellulose nanofibers (CNFs) were used as dispersing agent. The developed PDMS/CNF/CNT nanocomposite films were characterized for their electrical, mechanical, chemical, morphological, and surface-wetting properties. The results indicated that silane modified CNFs improves the dispersion of MWCNTs in PDMS improving the electrical conductance of the nanocomposite films. The electrical resistance of the nanocomposite film at 10 wt.% CNT to PDMS concentration was found to drop from ~80 k $\Omega$  to ~2.2 k $\Omega$  (approximately 97% reduction) when CNFs were introduced to improve the dispersion of the MWCNTs in PDMS. The nanocomposite film was found to withstand 2000 cycles of pulling forces producing strain up to 50% without showing significant differences in its electrical and mechanical properties. The nanocomposite film was then used to develop a sensing device to detect the flow rate of a fluid flowing through a channel and was able to detect flow rates as low as 100  $\mu$ L/s, which is comparable to many of the commercially available sensors. The electrically conducting PDMS elastomer-based flow rate sensor presented here has the potential to detect low flow rates in  $\mu$ L/s range which can be beneficial for biomedical applications. Besides that, the sensor is inexpensive and very easy to fabricate.

**Keywords:** *PDMS elastomer, cellulose nanofiber, electrically conducting PDMS, flexible electronics, fluid flow sensors*

# Electronic Properties of Solution-processed AgSPh and CuSPh

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## Abstract

Organic metal chalcogenides (OMCs) belong to the group of coordination polymers that have obtained significant attention due to the diverse range of their properties and structures, showing their potential for electronic applications. However, their poor solubility in common solvents is a primary limitation as they cannot be fabricated into thin films for device applications. This work aims to overcome the challenges associated with solution processing by employing amine-based solvents and to study the electronic and electrical properties of OMCs. In particular, we focus on silver benzenethiolate (AgSPh) and copper benzenethiolate (CuSPh) which contain metal-sulfur networks that have the potential to exhibit good electronic transport properties. The structural and morphological studies are investigated by X-ray diffraction (XRD) and atomic force microscope (AFM), showing that thin film-processing with the amine-based solvents can maintain the 2D structure of AgSPh with smooth film morphology. The electronic properties of thin films are investigated using various techniques, including photoelectron yield spectroscopy (PYS), ultraviolet-visible spectroscopy (UV-Vis), and Kelvin probe measurements (KP). The findings show that AgSPh and CuSPh behave as p-type semiconductors, featuring band gaps of approximately 3 eV. Remarkably, CuSPh exhibits conductivity of two orders of magnitude higher than that of AgSPh. These results provide a starting point for further study and development of electronic materials based on OMCs.

*Keywords: Organic metal chalcogenides (OMCs), Solution-processing, Electronic properties, Electrical conductivity*

# Exploring Interfacial Doping of Copper(I) Thiocyanate and Application in Thin-Film Transistors

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## Abstract

Doping plays a crucial role in modifying the electronic structures and properties of semiconductors. Among the emerging semiconductors, copper(I) thiocyanate (CuSCN) stands out due to its excellent hole transporting properties, high optical transparency, and cost-effective solution processability. Direct doping with an appropriate dopant has shown promise in improving the microstructure and passivating trap states particularly by eliminating hole-killing thiocyanate vacancies. As a result, thin-film transistors and solar cells based on doped CuSCN exhibit enhanced performance. However, the direct doping of CuSCN is hindered by limitations in dopant solubility as CuSCN is typically processed from unconventional nitrogen- or sulfur-containing solvents. In this work, we explore the interfacial doping by spin-coating potassium thiocyanate (KSCN) on the bottom contacts prior to the CuSCN layer deposition in staggered top-gate, bottom-contact thin-film transistors. When low concentrations (2 -10 mM) of KSCN are used, it facilitates crystal growth with a preferred orientation that promotes the hole-transporting Cu-S network in the plane of the substrate and a smoother surface. Consequently, the hole transport properties markedly improve, evident from an almost ten-fold increase in the hole mobility from  $0.011 \pm 0.004$  up to  $0.111 \pm 0.028$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>. Conversely, excessive KSCN treatment ( $\geq 12$  mM) induces the growth of discontinuous large crystals on the surface, resulting in surface inhomogeneity, higher leakage current, and reduced mobility. One significant concern is that the incorporation of KSCN leads to a larger hysteresis and increased off-current as seen in the transfer characteristic curves, which may point to the issue of ion migration. To overcome this, addressing and managing the ion mobility through the control of cationic size will be further investigated for elucidating this phenomenon, which could pave the way for a deeper understanding of this strategy and its use in practical applications.

**Keywords:** copper(I) thiocyanate, interfacial engineering, doping, thin-film transistors, semiconductor devices

# Ligand Modification in 2D CuSCN Co-Ligand Complexes

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## Abstract

Copper(I) thiocyanate (CuSCN) is recognized as a semiconductor with unique optical and electronic properties. Ligand modification represents an effective method for fine-tuning its characteristics. This approach impacts not only the structural and chemical attributes but also the optical and electronic properties. Such modifications hold the potential to enable new properties of CuSCN-based materials. As pyridine-coordinated CuSCN can result in two-dimensional (2D) structures that can retain the hole-transporting Cu-S network, we investigate the influence of electron-donating and electron-withdrawing substituents on the structure and subsequently the optical and electronic properties. CuSCN co-ligand complexes are synthesized as a series of pyridine derivatives with varying substituents at the 3-position (3-XPy where X = Cl, Br, H, or OMe). Through the coordination of CuSCN and 3-XPy, different structures can be generated, depending on the Cu:SCN:3-XPy ratio, and the resulting products are often mixed. In this work, we report a synthetic procedure that can reliably achieve a 1:1:1 ratio, enabling the controlled production of 2D coordination polymers [Cu(SCN)(3-XPy)]<sub>n</sub>. Furthermore, we employ single crystal X-ray diffraction (SC-XRD) to elucidate the crystalline structure of these complexes, while powder X-ray diffraction (PXRD), in conjunction with standard characterization methods including infrared (IR) spectroscopy, thermogravimetric analysis (TGA), and elemental analysis (CHNS), are employed to verify their phase and identity of the bulk materials. For the electronic properties, we observe a trend in the energy diagram of the complexes, measured from the pressed pellets. By varying the functional group at the 3-position of the pyridine ligand, we find that higher electron-withdrawing strength leads to a smaller band gap and a concomitantly higher electrical conductivity. With the strongest electron-withdrawing group, [Cu(SCN)(3-ClPy)]<sub>n</sub> shows a band gap of 2.79 eV and a conductivity of  $8.56 \times 10^{-8} \text{ S cm}^{-1}$ . The ligand modification holds significance for the design of novel semiconductors rooted in CuSCN-co-ligand complexes. Furthermore, the concept can be extended to other coordination polymers, thereby offering a promising avenue for the future development of novel semiconductors.

*Keywords: Copper(I) thiocyanate, coordination polymers, 2D structures, ligand modification*

## Surface Tension Assisted Gilding of Gold Leaf for Electrodes in Thin-Film Electronic Devices

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### Abstract

Electrodes are a vital part of any electronic devices. The most ubiquitous method in forming metal electrodes is the transfer of the source metal onto the substrates under high or ultra-high vacuum using techniques such as thermal evaporation or electron beam deposition. However, these methods require sophisticated equipment and lead to wastage of excess materials. Alternative methods utilizing metal particles (from nm to  $\mu\text{m}$ ) have been introduced. The particles are pre-synthesized and formulated into pastes or inks which can be deposited by coating or printing methods. Yet, the stability of the inks is of concern, and the conductivity of the resulting electrodes is typically lower than that of the source metal due to junctions or gaps between the particles. In this work, we develop a deposition method based on the gilding of metal leaf, which is commercially available for various metals. This method allows a low-cost technique for the creation of electrodes without the vacuum-based procedure while maintaining the continuity of the layer. The current key research questions are: (1) how to place the metal leaf on flat substrates with minimal creases which easily occur due to the small thickness ( $< 200\text{ nm}$ ); and (2) how to retain the leaf on the substrate that may have poor adhesion. By using a thin film of liquid on the substrate, the surface tension can assist in laminating the metal film onto the substrate while minimizing the roughness due to corrugation of the metal film. Additionally, introducing thickening agents, such as gelatin, can increase the surface tension, further reducing the roughness while also acting to promote the adhesion of the leaf onto the substrate. These steps allow the average roughness of the electrode surface to be reduced from  $\sim 200\text{ nm}$  to  $\sim 20\text{ nm}$  while covering a large area on the substrates.

*Keywords: Electrodes, Gold Leaf, Gold, Metallic Thin Films*



## Consolidation of Mn-Zn ferrite and sintering ceramic by cold sintering process

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### Abstract

MnZn ferrite powder ( $\text{Mn}_{0.8}\text{Zn}_{0.2}\text{Fe}_2\text{O}_3$ ) was synthesized through a co-precipitation method. The MnZn ferrite nanoparticles were cold sintered at 160 °C for 3h to form bulk samples. A liquid medium consisted of an oxalic acid solution and deionized water. The achieved relative densities of the sample were approximately 85%. The effect of the solvent was investigated, including phase analysis and crystallography using X-ray diffraction (XRD), as well as the magnetic properties using a vibrating sample magnetometer (VSM). XRD analysis showed MnZn ferrite phase for particles and bulk samples without any additional phases. Field emission scanning electron microscopy (FESEM) was used to study the microstructure of the sample and found that MnZn ferrite particles are connected to form the bulk structure. Magnetic properties by oxalic acid solution with maximum magnetic saturation value ( $M_s$ ) at 47.58 emu/g. Remanence ( $M_r$ ) 120.77 emu/g, Coercivity ( $H_c$ ) 19.63 kOe were magnetic behavior exhibited characteristics suitable for a versatile range of applications.

*Keywords: co-precipitation, cold sintering process, Mn-Zn ferrite, magnetic properties*

## PDMS-based Self-cleaning Nanocomposite Coatings for High Voltage Porcelain Insulators

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### Abstract

Porcelain insulators are widely used for providing electrical insulation in the high voltage transmission lines. However, due to the continuous exposure to various environmental factors, such as rain, high humidity conditions, dust, and other pollutant deposition, accumulation of contamination and formation of biofilms on these insulators is common which can lead to electrical leakages resulting flashover. Therefore, regular maintenance and cleaning of these porcelain insulators is necessary which involves high costs. In this research, the potential application of a polydimethylsiloxane (PDMS)-based nanocomposite is investigated as a superhydrophobic self-cleaning coating for porcelain surfaces. The nanocomposite was prepared using metal oxide nanoparticles and fluorocarbon silanes as filler materials in a PDMS matrix, which was simply sprayed on a porcelain surface to obtain the superhydrophobic properties with a static water contact angle higher than 155° and sliding angle as low as 2°. The surface showed excellent self-cleaning properties against dust, sand, soil, and graphite powders. The superhydrophobic coating also showed very good stability against a wide range of pH conditions (from pH 3 to pH 12) maintaining water contact angle within ±5%. Extended weathering tests up to 1000 hours demonstrated high stability of the nanocomposite superhydrophobic coating resulting nearly no change in the water contact angle values. The electrical insulation properties of the developed PDMS-based self-cleaning nanocomposite coating are currently under investigation and initial results are promising indicating their potential application in high voltage transmission lines leading to the reduction in the maintenance cost for the energy industries.

**Keywords:** self-cleaning, superhydrophobic, PDMS-based nanocomposite, electrical insulators, flashover

# Self-Healing and Electrically Conducting Photopolymer for Tactile Sensors

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## Abstract

The development of tactile sensors with high stretchability and self-healing utilizing additive manufacturing techniques for production has recently become attractive due to the convenience and direct fabrication of complicated sensor components for a number of applications, such as flexible electronics and sensors. However, most tactile sensors possess poor durability and a short lifetime as a consequence of microscopic damage induced by repetitive use. Herein, a flexible piezoresistive strain sensor with self-healing and 3D printing ability is proposed to address the aforementioned issues. The aim of the study is to develop a 3D printable photocurable resin employing the thiol-ene UV-curing reaction between thiol-modified and vinyl-terminated polydimethylsiloxanes (PDMS). Then, amino-modified and carboxyl-modified PDMS are induced into the resin in order to cause the rearrangement of the crosslinked networks, leading to the self-healing of the printed structure. Electrical conductivity is increased by employing carbon-based conductive fillers, namely carboxyl-functionalized multiwalled carbon nanotubes and carbon black. The stripes, 50 x 10 mm in size and 0.8 mm in thickness, created from prepared resin can be completely cured in less than 180 seconds with 405 nm UV light exposure, with very little stickiness on the sides of the stripes that are not directly exposed to UV light and contact with the surrounding environment. The produced resin has a high potential for use in the fabrication of free-form structures by digital light processing (DLP) 3D printing. The repetitive usage and self-healing capacities of sensors manufactured from the developed photocurable resin are evaluated by comparing the electrical and mechanical properties of the healed sensors against those the originals. Furthermore, the research further considers the photocurable polymer's properties like stretchability, electrical conductivity, and gauge factor, as well as demonstrate a proof-of-concept of a self-healing strain sensor fabricated from the additive manufacturing.

**Keywords:** Self-healing, Photopolymerization, Conductive Polymer Composite, 3D printing, Tactile Sensor

# Fabrication of Cement-rGO Nanocomposite for Enhancing Triboelectric Nanogenerator Performance.

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## Abstract

The cement-based triboelectric nanogenerator (TENG) is invented to harvest mechanical energy into electrical energy. The development of TENG has been rapidly progressed for self-powered harvesting and motion sensing applications owing to its great sensitivity, high energy harvesting performance, simple fabrication, and low cost. The cement-based TENG offers a large scale energy harvesting which covers various forms of mechanical energy. However, cement TENG shows relatively inferior TENG output performance. In this work, reduced graphene oxide (rGO) has been introduced to incorporate to cement to improve the electrical power generation of the TENG by enhancing charge capacitance of the cement composite due to its remarkable physical characteristics such as good electrical conductivity and high mechanical strength. The modification of cement with conductive rGO nanoparticles help improve dielectric constant which is essential for boosting the energy conversion performance of TENG. In addition, the compressive strengths of the cement-rGO composites are also studied. The morphology, crystal structure, dielectric properties of the cement-rGO composites are also investigated. The findings of this work show that the incorporation of rGO is able to magnify the electrical power generation as well as the improved mechanical strength of the cement-based TENG.

*Keywords: cement, reduced graphene oxide (rGO), triboelectric nanogenerator (TENG)*

## Fabrication of Cementitious materials for large scale energy harvesting and sensor application

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### Abstract

The triboelectric nanogenerator (TENG) is an emerging energy technology that utilizes the combination of triboelectrification and electrostatic induction to collecting wasted mechanical energy. This technology is particularly fascinating because TENG has the capability to generate electricity through the contact and separation of surfaces composed of different materials. Human step energy is one of enormous source of mechanical energy, which generally waste without being used. In this work, TENG is developed to harvest footstep energy from cement replacement materials, which have been considered as potential alternatives to cement materials replacement. Cement replacement materials offer various advantages, such as high mechanical strength, stability under thermal conditions, and great capability of harvesting the aforementioned mechanical energy with less carbon emissions. Herein, Cementitious pastes (CPs) are fabricated by combining fly ash with an alkali activator, a mixture of NaOH and Na<sub>2</sub>SiO<sub>3</sub> serving as a solution for geopolymerization reaction. The objectives of this study are to examine an optimal ratio of liquid to solid (L/S) used in the mixture and to fabricate CPs as triboelectric material for TENG to generate electricity from footsteps. The effects of the ratios on composite morphologies, microstructures, compressive strength, dielectric properties, and TENG performance are studied. The application of energy harvesting and motion sensing are demonstrated.

*Keywords: Cementitious pastes, Triboelectric nanogenerator, Mechanical energy harvesting*

## Development of Cement Replacement Materials for Energy Harvesting Application

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### Abstract

A triboelectric nanogenerator (TENG) is a device that can convert mechanical energy into electrical energy through the mechanism of electrification from frictional contact and electrostatic charge induction. In this work, cement replacement material or geopolymer is fabricated as a triboelectric friction material for TENG to harvest mechanical energy from human activities. Geopolymer material is synthesized from fly ash and alkaline binders including NaOH and Na<sub>2</sub>SiO<sub>3</sub>. The effects of the alkaline binder to fly ash ratios and binder ratios on formation of geopolymer and the TENG electrical outputs are studied. Experiments are conducted by using the alkali solution at 40, 45 and 50 % wt of fly ash and the ratio of NaOH to Na<sub>2</sub>SiO<sub>3</sub> at 1:1, 1:1.5 and 1:2. The smart energy floor fabricated from the geopolymer are demonstrate to harvest mechanical energy from human step. This research has proposed the development of new energy technology from green and environment friendly material.

*Keywords: Triboelectric Nanogenerator, Geopolymer*

## Effect of ZnO Nanoparticle Fillers on the Energy Generation Efficiency of Triboelectric Nanogenerator Fabricated Natural Rubber

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### Abstract

A triboelectric nanogenerator (TENG) is an energy-harvesting device that converts mechanical energy into electricity by using triboelectrification and electrostatic induction. In this work, ZnO nanoparticles are synthesized and used as filler material to improve the electrical output of natural rubber (NR) based TENG. The effect of ZnO particle size on TENG performance is investigated. The ZnO nanoparticles are prepared by the sol-gel method, which provides control over the particle size by adjusting the pH of the reaction. It is found that a higher pH value causes the ZnO nanoparticles with a smaller particle size resulting in the increased electrical output of TENG. This is attributed to the promotion of charge capacitance due to the well-distribution of small particle size of the ZnO nanoparticles. The NR-ZnO TENG with improved power output shows potential application as a power source for electronic devices.

*Keywords: Triboelectric Nanogenerator, Natural rubber, Zinc Oxide Nanoparticle*

# Modification of Activated Carbon by Acid and Plasma Treatments for Power Output Enhancement of Natural Rubber Based Triboelectric Nanogenerator

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## Abstract

Nowadays, the demand for energy is increasing and there are also environmental concerns on the consumption of fossil fuel. Therefore, development of environmentally friendly and sustainable energy sources is important. Triboelectric Nanogenerator (TENG) is a new emerging energy technology that converts mechanical energy in the environment into electricity based on a combination of contact electrification and electrostatic induction effects. In this research, TENG is fabricated for natural rubber (NR) material which is filled with activated carbon (AC) nanoparticles which are modified by acid and plasma treatment. The increased specific surface area and the presence of chemical functional group (C-N) on the surface of AC contribute to the environment of TENG electrical output. Therefore, this research provides key insight into the modification of AC for the development of TENG with high energy conversion performance.

*Keywords: Triboelectric Nanogenerator, Activated carbon, Acid, Plasma Treatment, Natural rubber*



## Synthesis of Carbon Nanotubes through Up-Cycling Hemp Waste by Chemical Vapor Deposition Method

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### Abstract

Since hemp has been legalized in Thailand, it is expected that the amount of hemp waste will increase along with hemp industry growth. In this study, hemp hurd waste was up-cycled into carbon nanotubes (CNTs) by chemical vapor deposition (CVD) where carbon bearing gas from pyrolysis of hemp hurds was used as carbon source and stainless-steel mesh (SS-304) was used as catalyst and substrate. The effect of temperature for pyrolysis ( $T_{\text{pyro}}$ ), temperature for CVD ( $T_{\text{CVD}}$ ) and catalyst surface treatment were studied. The synthesized CNTs were analyzed by Raman spectroscopy, field-emission scanning electron microscopy (FESEM) and transmission electron microscopy (TEM). It was found that for ethanol-washed catalyst, the condition of  $T_{\text{pyro}} = 800\text{ }^{\circ}\text{C}$ ,  $T_{\text{CVD}} = 800\text{ }^{\circ}\text{C}$  resulted in multiwalled-CNTs with average diameter of 318 nm with a ratio of G peak to D peak intensities ( $I_{\text{G}}/I_{\text{D}}$ ) of 0.94 in Raman spectra and the condition of  $T_{\text{pyro}} = 850\text{ }^{\circ}\text{C}$ ,  $T_{\text{CVD}} = 800\text{ }^{\circ}\text{C}$  resulted in multiwalled-CNTs with average diameter of 128 nm with  $I_{\text{G}}/I_{\text{D}}$  of 1.03. For 1 M HCl-washed catalyst, the condition of  $T_{\text{pyro}} = 850\text{ }^{\circ}\text{C}$ ,  $T_{\text{CVD}} = 800\text{ }^{\circ}\text{C}$  resulted in multiwalled-CNTs with an average diameter of 32 nm with  $I_{\text{G}}/I_{\text{D}}$  of 0.95. These results show the effect of temperature for pyrolysis, temperature for CVD and catalyst treatment on the quality and physical properties of the synthesized CNTs, suggesting the possibility of tailoring of physical parameters of CNTs through adjustment of mentioned growth conditions. Further details will be discussed in the presentation.

*Keywords: Carbon nanotubes, Hemp waste, Stainless-steel mesh, Chemical vapor deposition*

## Modification of Polydimethylsiloxane Using Yeast Cells for Enhancing Power Output of Triboelectric Nanogenerators

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### Abstract

A triboelectric nanogenerator (TENG) has been invented to harvest mechanical energy from the environment and convert into electricity based on triboelectrification and electrostatic induction effects. In general, polydimethylsiloxane (PDMS) is commonly used as a triboelectric material for fabricating TENG because the properties of the material are transparent, non-toxic, flexible, and hydrophobic, all of these properties are suited for manufacturing TENG. In this work, the electrical output of the triboelectric nanogenerator is enhanced by modifying PDMS using a fermentation reaction of baker's yeast. PDMS elastomer is mixed with yeast solution (YS) containing yeast cell and yeast extract and malt extract medium (YM) for undergoing fermentation reaction of yeast to produce carbon dioxide gas creating porous structures. The effects of YS content in PDMS on morphologies of PDMS films and TENG performance are investigated. The SEM images of the modified PDMS using YS reveals porous structures. It is found that the TENG fabricated from the PDMS modified by YS with a dilution of yeast solution creates a porous structure with a large pore size and can enhance the output performance of TENG. This paper indicates a simple and nonchemical method for creating a porous structure PDMS to enhance the electrical performance of TENG.

*Keywords: Triboelectric nanogenerator, Polydimethylsiloxane, Yeast*

## Fabrication of Natural Rubber Films for Particulate Matter Filter and Energy Harvesting Applications

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### Abstract

Human activities in their living environment are related to energy consumption, which could cause the air pollution that affect the environment and human health, in particular, the particulate matter (PM). The development of clean power source that does not cause the air pollution and exhibit PM removal property would be crucial for recent years. In this work, a triboelectric nanogenerator (TENG) is fabricated from porous natural rubber composite which is able to convert mechanical energy into electricity and filter PM. The natural rubber composite with porous structure is synthesized. The effects of the porous structure on the energy conversion efficiency and PM removal efficiency are studied. It was found that the TENG fabricated from natural rubber composite can generate electricity with the highest power density of 4.6 W/m<sup>2</sup> and has the efficiency of PM removals of about 50%. This is attributed to the large contact surface area of porous structure and good dielectric property of natural rubber composite. This study provides key insight into the fabrication of porous natural rubber for the development of future power source and air filter which is clean and sustainable.

*Keywords: Triboelectric Nanogenerator, Air Filter, Particulate Matter Removal, Natural Rubber, Cellulose*

# Fabrication of Cellulose Paper from Sugarcane Leaves Filled with ZnO Nanoparticles/Chlorophyll Nanocomposites for Triboelectric Nanogenerator Application as a Micro/Nano Electronic Power Source

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## Abstract

In research, the cellulose paper is synthesized with cellulose fibers (CF) from sugarcane leaves, which exhibits excellent properties, including biodegradability, recyclability, and excellent mechanical strength as well as flexibility. Hence, cellulose papers (CP) are widely used to fabricate an energy harvesting device called a triboelectric nanogenerator (TENG) that converts mechanical energy into electricity based on contact electrification and electrostatic induction effects. CP is synthesized and modified by adding Zinc Oxide (ZnO) nanoparticles with chlorophyll extracted from spinach leaves to improve the TENG performance. The effect of ZnO nanoparticles with chlorophyll loading on the electrical output of the fabricated CP TENG is investigated. It is found that ZnO nanoparticles with chlorophyll can increase electrical output of TENG by the promotion of triboelectric charge capacitance. The generated electricity can charge a capacitor which is then used as the power source for small, electronics devices. This work has proposed the use of sugarcane leaves which is one of the main agricultural waste to develop a clean and sustainable power source.

*Keywords: cellulose fibers, triboelectric nanogenerator, Zinc Oxide nanoparticles, chlorophyll*

## 1,2,3-Triazole-phenanthroimidazole isomeric derivatives as hot exciton emitters for high-efficiency non-doped blue OLEDs

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### Abstract

Herein, we report the design and synthesis of novel blue emissive hot exciton molecules using a D-A system of phenanthroimidazole (PI) as a weak donor and 1,2,3-triazole (TAZ) as an acceptor. To fine-tune the acceptor property, PI was linked to different positions of the 1,2,3-triazole moiety thereby forming two isomeric molecules of 2-(4'-(1,4-diphenyl-1H-1,2,3-triazol-5-yl)-[1,1'-biphenyl]-4-yl)-1-phenyl-1H-phenanthro[9,10-d]imidazole (PI-5TAZ) and 2-(4'-(1,5-diphenyl-1H-1,2,3-triazol-4-yl)-[1,1'-biphenyl]-4-yl)-1-phenyl-1H-phenanthro[9,10-d]imidazole (PI-4TAZ). PI-5TAZ and PI-4TAZ in thin film exhibit blue emissions peaked at 450 nm and 456 nm with PLQYs of 34% and 50%, respectively. The solvatochromic studies and theoretical calculations support that PI-5TAZ and PI-4TAZ are hot exciton emitters with a narrow gap ( $< 0.2$  eV) between  $T_3$  and  $S_1$  promoting RISC from  $T_3$  to  $S_1$  via the “hot exciton” channel and a large splitting between  $T_2$  and  $T_1$  inhibiting internal conversion from  $T_2$  to  $T_1$ . They are successfully applied as non-doped emitters in OLEDs. Both devices exhibit intense blue emissions (445-463 nm), low turn-on voltages (3.0-3.2 V), and superior electroluminescent (EL) performances ( $\text{EQE}_{\text{max}} = 5.30\text{-}7.00\%$  and  $\text{CE}_{\text{max}} = 4.89\text{-}7.36 \text{ cd A}^{-1}$ ). Particularly, PI-4TAZ-based OLED emits blue EL emission peaked at 463 nm (CIE coordinates of (0.15, 0.14) with a high  $\text{EQE}_{\text{max}}$  of 7.00% and a high exciton utilization efficiency (EUE) of 70%. Our results establish that by taking advantage of molecular tuning of 1,2,3-triazole-phenanthroimidazole derivatives, ambipolar blue hot exciton emitters, as well as non-doped blue OLEDs with high performance, could be realized, which has a promising prospect for the displays and lighting in the future.

**Keywords:** 1,2,3-Triazole; Phenanthroimidazole; Hot exciton; Blue emitter; OLED

## Efficient non-doped emitter with dual hybridized local and charge-transfer characteristics for organic light-emitting diodes

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### Abstract

Herein, we report a new design of a dual hybridized local and charge-transfer (HLCT) fluorescent molecule, namely SBF-2BzFC, as an efficient non-doped emitter for organic light-emitting diodes (OLEDs). SBF-2BzFC is assembled by conjugated linking two HLCT fragments of 7-(4-(carbazol-*N*-yl)phenyl)benzothiadiazole (BzFC) with a 9,9'-spirobifluorene (SBF) core. The theoretical calculations and photophysical studies approve its HLCT excited-state character with a strong yellowish-green fluorescence emission and a high solid-state photoluminescence quantum yield of 70%. Moreover, the molecule also exhibits excellent thermal stability and ambipolar charge-carrier-transporting properties with a decent balance of mobility of electron ( $1.95 \times 10^{-5} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ) and hole ( $4.84 \times 10^{-6} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ) which are appropriate for device fabrication. SBF-2BzFC is successfully utilized as a non-doped emitter in OLEDs. This device achieves excellent electroluminescence (EL) performance with a high brightness of  $20150 \text{ cd m}^{-2}$ , a maximum external quantum efficiency ( $\text{EQE}_{\text{max}}$ ) of 6.68%, a maximum current efficiency ( $\text{CE}_{\text{max}}$ ) of  $7.35 \text{ cd A}^{-1}$  and a high exciton utilization efficiency (EUE) of 47%.

**Keywords:** Dual hybridized local and charge-transfer (HLCT), Non-doped emitter, 9,9'-Spirobifluorene, benzothiadiazole, Organic light-emitting diode

# Nanoscale precision on a budget: lab-constructed super-resolution fluorescence microscopy for particle tracking

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## Abstract

In this study, we introduced an affordable super-resolution fluorescence microscopy setup, designed specifically for nanoscale precision in single particle tracking. Priced below \$10k, our lab-built solution is a significant departure from the conventional commercial inverted epifluorescence microscopes, which often cost around \$120k. Despite the stark difference in cost, our design does not compromise on performance. By strategically sourcing components from diverse suppliers, our setup incorporates a 450-nm excitation laser, specific optics, an industrial-grade CMOS camera, and highly luminescent polymers. Preliminary evaluations showed the blue excitation light, shaped by a rotating diffuser, projects an intensity of about 100 W/cm<sup>2</sup> on the sample plane. The camera is capable of capturing video at 55 Hz with a quantum efficiency of 70% and a minimal readout noise of 3 electrons. We employed custom MATLAB simulations to refine optical parameters and determine localization precision, focusing on any deviations from the fluorescence centroid. Through these simulations, particle mobility was assessed using the mean-squared displacement method. By adjusting specific parameters like quantum yield and camera gain, our innovative setup reached an impressive localization uncertainty below 10 nm, making it suitable for tracking individual fluorescent molecules. This groundbreaking and cost-effective microscopy setup aims to democratize access to single particle tracking. With the prohibitive costs of commercial options often being a barrier, our findings offer a more accessible, yet equally precise, microscopy solution for the scientific community.

*Keywords: Super-resolution fluorescence microscopy, single particle tracking, localization precision*

## Experimental Study of Electrowetting on Dielectric Combine with Electrochemical Sensor for Depressive Substance Analysis

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### Abstract

This research investigated a screen-printed electrowetting on dielectric (EWOD) microchip for depressive substance analysis using a two-part design, a T-junction EWOD containing all the two layers which were a silver electrode and a polydimethylsiloxane (PDMS) dielectric layer. The electrochemical sensor part was at the end of the T-junction EWOD. Three detectors comprised a screen-printing electrode which were graphene/carbon working and counter electrodes, and a silver/silver chloride reference electrode. Both parts of electrode were fabricated using a layer-by-layer screen printing method. The PDMS layer was fabricated using the spin coating method. The electrochemical sensors perform cyclic voltammetry analysis for substances associated with depression. The results showed that electrochemical sensor was a high possibility for depressive substance analysis.

*Keywords: Electrowetting on dielectric (EWOD), electrochemical senso, graphene/carbon paste, depressive substance*



## A Plastic Based Digital Microfluidic Microchip by Screen Printing

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### Abstract

This research study about digital microfluidic microchip integrate with electrochemical sensor on plastic based designed and experimental studied for chemical analysis. For the design, the microchip was designed with H-junction electrowetting on dielectric (EWOD) configuration and the electrochemical sensor at the end of the junction for the electrochemical analysis comprising with three detectors including silver/silver chloride reference electrode, graphene/carbon counter and graphene/carbon working electrodes. H-junction EWOD and electrochemical sensor were fabricated by screen printing technique. For experimental study, the microchip integrate with electrochemical sensor was tested with cyclic voltammetry for different concentration of substance. For analysis, digital microfluidic microchip was demonstrated to test for the electrochemical sensor for minimal reagent consumption. The results revealed about performance detection of a plastic based EWOD microchip with integrated electrochemical sensor that can be used for automated chemical analysis.

*Keywords: Digital Microfluidic microchip, electrowetting on dielectric (EWOD), electrochemical sensor, graphene/carbon paste*

# Robust, Stretchable, Recyclable and Healable Supramolecular Elastomers via Structural Functional Region Strategy and Metallic Cross-Linking

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## Abstract

With the development of technology, incorporating both high mechanical strength and exceptional self-healing capability into polymeric elastomers offers appealing possibilities in fields such as electronic skin, soft robotics, and electrical devices. Nevertheless, achieving a simultaneous enhancement of these two properties remains a significant hurdle due to the intricate balance required between strong and weak dynamic bonds. Here, we develop a material with self-healing capability and great strength mechanical properties via a one-pot polycondensation reaction between bis(3-aminopropyl)-terminated poly-(dimethylsiloxane) (PDMS) with varying molecular weights and isophorone diisocyanate (IPDI), followed by being crosslinked with Aluminum acetylacetonate ( $\text{Al}(\text{acac})_3$ ). The polymeric elastomer system exhibits two distinct functional regions due to the presence of PDMS with different molecular weights. These regions are characterized as low density and high density hydrogen bond functional regions. In the low density hydrogen bond functional regions, the chain segments possess higher mobility, which enhances the material's self-healing capability and enables efficient energy dissipation upon external impact. On the other hand, the high density hydrogen bond functional regions contain chain segments with a higher energy barrier, imparting rigidity to the network and leading to excellent mechanical properties in the material. Furthermore, the incorporation of  $\text{Al}(\text{acac})_3$  as the crosslinker introduces strong dynamic bonds, resulting in robust molecular networks. Owing to these design strategies, PUIP\_S8L2-Alac exhibits excellent transparency (98.5%), high tensile strength (4.58 MPa), and good healing ability under moderate temperature.

*Keywords: polymeric elastomers, self-healing, mechanical robustness, metallic cross-linker*

# Aluminum Acetylacetonate-Initiated Metal-Ligand Coordinated Elastomers Exhibiting Stretchability, Self-healing and Flame-Retardancy for Human Motion sensing

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## Abstract

The field of self-healing materials based on metal-ligand coordination has made significant progress, but has been hindered by the reliance on transition or rare earth metal ions and their limited potential for mass production. Herein, aluminum, being the most abundant metal element in the Earth's crust, offers immense potential for the development of aluminum metal ion-coordinated self-healing elastomers, enabling widespread application and large-scale production. However, previous attempts to create  $\text{Al}^{3+}$ -based self-healable and stretchable materials have been restricted by their inadequate performance. In this study, we address this challenge by comparing the use of acetylacetonates ( $\text{Acac}^-$ ) and chlorides ( $\text{Cl}^-$ ) as anions in  $\text{Al}^{3+}$ -coordinated metal salts, combined with phosphorus-containing small molecules (3N2AP), to fabricate two series of elastomers:  $\text{Al}_{\text{ac}}\text{-3N2AP-PTD}$  and  $\text{Al}_{\text{Cl}}\text{-3N2AP-PTD}$ . Our findings demonstrate that  $\text{Al}_{\text{ac-0.25}}\text{-3N2AP-PTD}$ , which incorporates  $\text{Acac}^-$  into the polymer matrix, exhibits exceptional properties, including high transparency (96.9%), remarkable toughness ( $16.56 \text{ MJm}^{-3}$ ), and efficient self-healing (92% healing efficiency within 6 h). In contrast,  $\text{Al}_{\text{Cl-0.25}}\text{-3N2AP-PTD}$  shows relatively lower transparency (86.1%), self-healing capability (91% healing efficiency within 48 h), and toughness ( $5.71 \text{ MJm}^{-3}$ ). Furthermore, we incorporate electrochemical polymerization method to fabricate polypyrrole(ppy)-coated  $\text{Al}_{\text{ac-0.25}}\text{-3N2AP-PTD}$ , demonstrating a stable, self-healable and stretchable strain sensor for human-motion sensing. These results underscore the significant advantages of  $\text{Al}_{\text{ac-0.25}}\text{-3N2AP-PTD}$  for potential applications in transparent, self-healing materials with enhanced comprehensive properties.

**Keywords:** polymeric elastomers, self-healing, stretchable, dynamic metal-ligand coordination, human-motion sensing,

# Electrical and Sensing Properties of Gold-Decorated Zinc Oxide Nanoflowers

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## Abstract

In this study, gold nanoparticles (Au NPs) were decorated on the surface of ZnO nanoflowers to enhance electrical and gas-sensing properties of ZnO. The ZnO nanoflowers were synthesized by solvothermal method using zinc acetate dihydrate as reactant, and sodium citrate dihydrate as a chelating agent. The white powder of ZnO nanoflowers was transform to pink powder after adding Au NPs. The crystal structure and surface morphology of composite materials were investigated. The results confirm the decoration of Au NPs on the surface of ZnO nanoflowers. The sensing devices were fabricated by spin-coating Au/ZnO precipitate on an aluminum interdigitated electrode. The electrical conductivity was investigated under dark and UV light illumination at room temperature. The conductivity of Au/ZnO exhibit lower than that of pristine ZnO. Under UV light illumination, the conductivity of both pristine ZnO and Au/ZnO increases with increase of UV light intensities. Additionally, the sensor-based Au/ZnO exhibit hight sensitivity to ethylene gas than those of pristine ZnO.

*Keywords: zinc oxide, gas sensor, UV light illumination, Au NPs-decorated ZnO*

## Effect of CoPc Thickness on Optical and Electrical Properties of CoPc/IGZO Hybrid Thin Film

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### Abstract

Hybrid thin film is a new strategy of high-performance gas sensor platform. In this work, we investigate the optical and electrical properties of CoPc/IGZO hybrid film sensor with varying CoPc thickness and operating under light illumination. The sensing devices were prepared by spin coating IGZO on SiO<sub>2</sub> substrate, then evaporating aluminium interdigitate electrodes, and depositing CoPc film on the top of electrodes. The thickness of IGZO layer was fixed at 10 nm. To investigate the effect of CoPc layer on devices properties, the CoPc thickness was varying from 20 nm up to 100 nm, which was prepared by thermal evaporation. The results show that the IGZO film exhibit absorption wavelengths below 390 nm, while the CoPc film exhibit multiple absorption peaks at wavelengths of 284 and 325 nm, 618 and 687 nm corresponding to B-band and Q-band, respectively. The current-voltage characteristics of the IGZO and CoPc/IGZO films in the dark conditions exhibit Schottky behaviour. When illuminated the light emitting diode with a wavelength of 390 nm, the electrical characteristics of the devices transform to Ohmic characteristic. The CoPc/IGZO devices exhibits decreases in photocurrent as the thickness of the CoPc film increases. The gas sensing characteristics of CoPc/IGZO films under light illumination were also studied for optimizing the highest performance of nitrogen dioxide gas detection.

*Keywords: IGZO, CoPc, Hybrid thin film, IV characteristics, Photo current*

# New Biosensor Modalities Through Surface Modification with Nanoscale DNA Origami Structures

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## Abstract

Electrochemical biosensors offer great promise in meeting the diagnostic demands of modern healthcare where the ability to screen for common diseases at low cost will become increasingly important. In our laboratory we have been working on the development of biosensor systems using gold electrodes and self-assembled monolayers (SAMs). These systems offer high sensitivity (nanomolar to femtomolar) for a range of analytes but can suffer from problems with spatial organization, stability and manufacturability. With overcoming these shortcomings in mind, we have been investigating electrode surfaces modified with DNA origami. This material is attractive for a number of reasons which include: it's ability to give exquisite spatial control, ease of design, ready attachment of functional groups and other biological molecules and its scalability through use of existing oligonucleotide production techniques. In this talk, two systems will be described, the first a DNA zipper featuring a series of pH responsive lock structures and the second a DNA origami tile designed specifically to boost the signal in an impedance based nucleic acid detection assay. The talk will show how the DNA zipper is able to measure solution pH via changes in the electrochemical signal arising from switching from open and closed states at different pH ranges and describe how a sensitive assay (low picomolar LOD) for the oxacillin resistance gene *oxa1* was developed using the origami tile structure. Finally, our work with nanoelectrode systems will be introduced where we have so far studied the formation of SAM layers on platinum nanoband electrodes. These nanoscale electrode devices offer exceptional signal to noise and other performance advantages over conventionally scaled electrodes. Our future aim is to combine the DNA origami surface modifications with nanoscale electrode devices.

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*Keywords: electrochemical biosensors, impedance, self-assembled monolayers, DNA origami, nanoscale electrodes*

**Short Bio: Prof. Damion Corrigan**

Damion Corrigan is the LGC Professor in Measurement Science for Health and leads the Centre for Advanced Measurement and Health Translation - a joint initiative with the National Measurement Laboratory (NML) at the Laboratory of the Government Chemist (LGC), the University of Strathclyde and NHS Lanarkshire. The aim of the centre is to develop cutting edge interdisciplinary projects which drive new healthcare and measurement science R&D in Scotland.

Using core expertise in electrochemical sensing, analytical chemistry and device fabrication Damion's research aims to develop improved diagnostic tests for clinically important conditions such as, drug resistant bacterial infections, COVID-19, sepsis, cancer and epilepsy. The group work on device fabrication, surface functionalisation, bioconjugation, sample handling, measurement techniques and assay development for a range of sensor systems, from high value microfabricated arrays, to wearables and through to low cost devices for use in resource limited settings. In addition to academic research, translational activity is an important aspect of the group's work because they are keen to ensure that developments from the lab ultimately find real world application. As a result of this, Damion is the founding Director of Aureum Diagnostics and a co-founder of Microplate Dx and remains involved in their ongoing R&D activity. His work is often highly interdisciplinary involving industrial partners (e.g. GSK, National Nuclear Laboratory, AstraZeneca, Lifescan, Aptamer Group, FlexMedical Solutions, Biotangents and other SMEs) and projects rely on close collaboration with other academics, including: clinicians, experts in fluidics/sample handling, microbiologists, neuroscientists, electrical engineers and chemists.

Damion is a Fellow of the Royal Society of Chemistry (FRSC). He co-chairs the Measurement Science Institute for the Community of Analytical Measurement Science - UK (CAMS-UK), is a panel member of the UKRI Interdisciplinary Assessment College and sits on the National Physical Laboratory Industrial Committee on Biosensors.

## Advanced Nanomaterials for Cancer Detection and Phototherapy using Light-responsive Molecules

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### Abstract

Imaging-guided cancer therapy is a therapeutic technology that rely on nanoparticles with two functions, including, 1) fluorescent imaging and 2) cancer therapeutic function. The first function can be acquired from emissive aggregation-induced emitting (AIE) agents, the compounds that exhibit bright fluorescent emission in NIR region in the aggregated state or inside the nanoparticle core. The second function can be obtained from photosensitizers (PS) that can generate heat or reactive oxygen species (ROS) upon NIR light illumination referring to photothermal therapeutic (PTT) agents and photodynamic therapeutic (PDT) agents, respectively. In this presentation, we propose to show our recent results based on; i) AIE-based nanoparticles for cancer imaging, ii) PTT nanoparticles, and iii) PDT nanoparticles based on aza-BODIPY core for cancer ablation via imaging-guided phototherapy concept using heat and reactive oxygen species (ROS), respectively. The biological applications of all nanoparticles have been studied in cell-based assays (in vitro), an avian embryo model (in ovo), and a murine model (in vivo) to confirm their potentials for future clinical uses as new imaging-guided therapeutic agents.





**Short Bio: Kantapat Chansaenpak, Ph.D**

**Senior researcher**

Responsive NanoMaterials Research Team

Responsive Materials and NanoSensors Research Group

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**Work Experience**

- |                   |   |
|-------------------|---|
| 01/2022 – present | Senior researcher at National Nanotechnology Center, National Science and Technology Development Agency (NSTDA), Pathum Thani, Thailand |
| 10/2016 – 12/2021 | Researcher at National Nanotechnology Center, National Science and Technology Development Agency (NSTDA), Pathum Thani, Thailand        |
| 08/2015 – 08/2016 | Postdoctoral Research Associate at University of North Carolina--Chapel Hill, NC, USA (Advisor: Prof. Zibo Li)                          |
| 08/2010 – 08/2015 | Graduate Teaching/Research Assistant at Texas A&M University--College Station, TX, USA (Advisor: Prof. François P. Gabbaï)              |

**Honors/Awards**

- 2023 15th Austrian Leadership Program (ALPs-15) participation at Vienna/Innsbruck, Austria, privately invited by the Austrian Embassy in Bangkok
- 2023 Outstanding research award from the National Research Council of Thailand (NRCT) for the research entitled: Strategies to target cancer therapy using near-infrared fluorescent dyes.
- 2022 Silver medal from the international trade fair ideas inventions new products (iENA), Nuremberg, Germany, for the invention Mn Sense: Manganese ion test kit and DuoEye Reader.
- 2022 FIRI Award for the best invention from the First Institute of Researchers and Inventors in I.R. Iran for the invention Mn Sense: Manganese ion test kit and DuoEye Reader.
- 2022 Outstanding research award from the National Research Council of Thailand (NRCT) for the research entitled: Aza-BODIPY encapsulated polymeric nanoparticles as effective nanodelivery system for photodynamic cancer treatment
- 2021 Outstanding research award from the National Research Council of Thailand (NRCT) for the research entitled: Near-infrared fluorescent pH responsive probe for targeted photodynamic cancer therapy
- 2020 Excellent dissertation award from the National Research Council of Thailand (NRCT) for the dissertation entitled: Organoboranes as 18F Fluoride Anion Captors
- 2015-2016 Postdoctoral Fellowship at Biomedical Research Imaging Center, University of North Carolina--Chapel Hill
- 2003-2015 Full scholarship from the Development and Promotion of Science and Technology Talents project (DPST)
- 2014 Travel award from Office of Graduate and Professional Studies, Texas A&M University
- 2013 63<sup>rd</sup> Lindau Nobel Laureate Meeting participation at Lindau, Germany, selected and supported by National Science and Technology Development Agency of Thailand (NSTDA)
- 2013 Travel award from World Molecular Imaging Congress
- 2012 Travel award from Cotton Memorial foundation
- 2009 Excellent Academic Record, Chiang Mai University (GPA: 3.91) 2006 Professor Dr. Tab Nilanidhi foundation award

## Emerging Nanosensors for Cancer and Metabolic Disease Screening: A Journey from Research to Regulatory Milestones

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### Abstract

Moving from research to real-world applications in medicine is a challenging journey, filled with both technical and regulatory obstacles that can discourage many researchers. In this presentation, I will provide a detailed overview of our group's work on specialized nanosensors, designed for liquid-biopsy cancer screening and early detection of metabolic diseases like diabetes and chronic kidney disease. We will focus on the development of nanosensors that can detect miRNA and lncRNA, which are important markers in cancer diagnostics. Additionally, I will discuss nanosensors aimed at the early identification of diabetes and chronic kidney disease. I will walk the audience through the entire course of our research, from its initial concept to achieving ISO13485 qualification for select devices. The presentation will conclude with the most recent updates on our newest nanosensor, which is currently seeking regulatory approval.

### References

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- 3) Ultrasensitive Detection of MicroRNA in Human Saliva via Rolling Circle Amplification Using a DNA-Decorated Graphene Oxide Sensor. *ACS omega* 8 (17), 15266-15275.
- 4) Isothermal detection of lncRNA using T7 RNA polymerase mediated amplification coupled with fluorescence-based sensor. *Analytical Biochemistry* 629, 114212.

**Short Bio: Dr. Deanpen Japrun, Dphil (Oxon), BSc, MSc, MRSC**

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National Nanotechnology Center, National Science and Technology Development Agency

**Education**

2006-2010 D.Phil. (Chemical Biology), University of Oxford, United Kingdom  
2000-2004 M.Sc. (Biochemistry), Mahidol University, Thailand  
1996-2000 B.Sc. (Medical Technology, Honors), Chulalongkorn University, Thailand

**Awards**

2021 Department of Medical Science (DMSc) Award 2021  
People Choice Award from Pinching competition organized by LIF, RAEng, Newton Fund  
2020 Leaders in Innovation Fellowships (LIF) Program, The Royal Academy of Engineering (RAEng),  
Newton Fund  
2020 Diabetes Association of Thailand activity award 2019 (The winner Award 2019)  
2019 Silver Medal in medical device in “International Exhibition of Inventions of Geneva”  
2019 Emerging investigator series from Analyst, RSC  
2019 National Research Council of Thailand Research Award in Medical science 2018  
2018 Diabetes Association of Thailand activity award 2018 (The winner Award 2017)  
2017 Diabetes Association of Thailand Activity Award 2016 (Honorable Mention Award)  
2017 Department of Medical Sciences (DMSC) award (first runner)  
2015 The Royal Society Chemistry (UK) Research Fund Award 2015  
2014 The Royal Society Chemistry (UK) Research Fund Award 2014  
2014 National Research Council of Thailand Fund Award 2014  
2011 Balliol college scholarship, University of Oxford  
2006 The Royal Thai Government Scholarship 2006-2010

**Experiences**

2018-Present Research Group Director of Responsive Material and Nanosensor Research Group  
2014-Present Co-founder of Japrun Foundation for Rural Education (JFRE)  
2015-2022 Royal Society of Chemistry (RSC, UK) representative in Thailand  
2016-2018 Group leader at Nano-molecular Target discovery laboratory,  
National Nanotechnology Center (NANOTEC, Thailand)  
2012-2015 Researcher at National Nanotechnology Center (NANOTEC, Thailand)  
2013 Asian Research Network (ARN) Summer Camp, Institute of Nano Science and Technology,  
Hanyang University, South Korea  
2010-2012 Postdoctoral researcher at Department of Chemistry, Imperial College London, UK  
2000-2006 Research Assistant at National Center for Genetic Engineering and  
Biotechnology (BIOTEC), National Science and Technology  
Development Agency (NSTDA), Thailand

# Micromotors in Nanomedicine: Biosensing on the Fly for Clinical Diagnosis

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## Abstract

Micromotors represent one of the most exciting horizons in micro and nanotechnologies. The utilization of self-propelled micromotors in (bio)chemical assays has led to a fundamentally new approach where their continuous movement around the sample and the mixing associated effect, all this as a collective behavior, greatly enhances the target-receptor interactions and hence the performance of the bioassay [1-3].

In our lab, we are focusing on the design and development of micromotors which are constituted by (nanostructured) layers (tubular-based shape) and particles (Janus-based shape) that confer them self-propulsion using (photo)-catalytic propulsion and magnetic guidance with compatibility in biological media due its tremendous significance, as it has been critically reviewed [4-6]. They also smartly incorporate nanomaterials and molecular recognition-based functionalization to obtain sensitivity and exquisite selectivity on board using electrochemical and fluorescence detection approaches. Also, we have explored the coupling of micromotors even with electrochemical microfluidics. In our experience, we humbly found that micromotor technology is an attractive alternative to performing fast, reliable bioassays and diagnostic testing, especially when an extremely low volume of samples is available, or the analysis must be performed in a micro-size environment.

This Keynote will discuss selected micromotors-based bioassays with potential in diagnostics and some future directions. But ultimately, we try to find the potential future of micromotors in nanomedicine.

## ACKNOWLEDGMENT

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- [6] R. Maria Hormigos, B. Jurado-Sánchez, A. Escarpa, *Anal Bioanal Chem* 414 (2022) 7035–7049

*Keywords: Surface enhanced Raman scattering (SERS), gold nanorod, biomarker, cancer, diabetes mellitus*



**Short Bio: Jesús Alberto Escarpa Miguel**

Dr. Alberto Escarpa is a Full Professor of Analytical Chemistry at the University of Alcalá (UAH). He is the leader and founder (in 2003) of the “Analytical Miniaturization and Nanotechnology” (MINYNANOTECH) research group. His main research interests are designing and developing nanomaterials-based (wearable) (bio)sensors, electrochemical microfluidics, lab-on-a-chip and organ-onchip technologies, and artificial micromotors. He has co-authored more than 200 articles in leading international peer-review journals, 6 patents, and 11 book chapters, yielding an h-index of 50. He has recently been included in the top 2% (1% position in the ranking) of most cited chemists in the world by Stanford University (2020,2021). His works have been highlighted several times in top journals such as *Angewandte Chemie International Edition*, *Chemical Science*, *Lab on a Chip* or *Analytical Chemistry*, and social media (*Chemical World*, *RSC*; *Separations Now*, *Wiley* and *C&EN news ACS*, *Nanowerk*). He has edited and authored several books including “*Miniaturization of analytical systems: principles, designs, and applications*” (Wiley, 2009), “*Food Electroanalysis*” (2015, Wiley), and “*Carbon-based Nanomaterials in Analytical Chemistry*” (RSC, 2018). He is a member of the Editorial Board of *Analytical Chemistry*, *Analysis & Sensing*, *Applied Materials Today*, *Journal of Nanobiotechnology*, and *Electrophoresis*. He has been Associate Editor for *RSC Advances* (2015-2019) and Associate Editor (2018-2019) for *Microchimica Acta*. Since 2019, he is Editor in Chief for *Microchimica Acta*. He has given about 40 invited lectures at the most prestigious forums of micro and analytical nanotechnologies. He has received several awards such as the NATO Fellowship to perform postdoctoral research at the New Mexico State University (USA) in 2001, the “Young Investigator Award” by the University of Alcalá in 2003, the International Dropsens Award for “Best research work in applied electroanalytical chemistry” (finalist) in 2015. He served as a visiting professor in international Universities and research centers such as the University of California San Diego (USA) and the International Center for Young Scientists in the National Institute for Materials Science (Tsukuba, Japan). He has also been a visiting professor at Buenos Aires University. He is currently a scientific partner at Nanorobots Research Center (Prague, CR) and a visiting professor at Prince of Songkhla University (Thailand). Prof. Escarpa is also a member of the Collegium of the Ph.D. in Food Science at Teramo University (Italy). He has also supervised 20 Doctoral Thesis (15 with International Mention) with 20 awards and honors (10 Extraordinary Awards, 5 Awards for the Best Thesis in Chemistry of the RSEQ-STM, 1 Lilly-RSEQ 2020, 1 National Award for the best Thesis of Health Sciences of Funcas, 3 Award for the Best Thesis of the Society of Condueños). The “Excellence Award in Doctoral Thesis Supervision of Sciences in 2021” award has recognized such excellent mentoring activity at the University of Alcalá. Since 2018, he is a collaborator of the Spanish State Research Agency, CTQ (Chemistry) area of the Coordination, Evaluation, and Technical Scientific Monitoring Division.

# Carbon Nanotubes-Modified Sustainable Sensors for Advanced Practical Electroanalysis and Effective Enzyme-Based Biosensing

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## Abstract

Carbon nanotubes (CNTs) were discovered in their single-wall version in the early 1990ies by Iijima and Ichihashi and they are hollow cylinders of rolled up individual or stacked graphene sheets with nanometer diameters. A superb mechanical strength combined with ultrahigh flexibility, a remarkable chemical inertness on the one hand and the aptness for functional group addition on the other, and finally a great electrical conductivity in tube direction are the outstanding properties that made CNTs a high-tech material of the modern age. Reported industrial and research applications range from the utilization in energy store and sensor devices to the incorporation as strengthening component in parts of cars, boats, planes and trains and sporting goods, explorations as nanoporous fillings of water filters, conductive thin-film adaptations of electronic platforms, the responsive units of actuators, and placement as effective electromagnetic shields. In this conference contribution discussed will be a selection of own explorations of CNTs as highly beneficial functional modification of the surfaces of electrochemical detectors and amperometric enzyme biosensors. Particular attention will be paid to the role that the graphitic nanomaterial plays in the reach of the desired improvement of electrochemical analyte signaling.

### Short CV

Albert Schulte received the Ph.D. degree from the University of Münster, Münster, Germany, for the development of carbon fiber-based microelectrodes for advanced electroanalysis and tailored probe microscopy. Since 2017, he is Analytical Chemistry Professor in the School of Biomolecular Science and Engineering (BSE) of the Vidyasirimedhi University of Science and Technology (VISTEC). His cross-disciplinary group research at VISTEC is tackling advancements of (bio-) electroanalysis for biomarker, pollutant, food nutrient/contamination and drug screening with special focus placed on the automation, miniaturization, simplification, and greening of the applied electroanalytical tools and procedures. And greening and improving enzyme biosensors through immobilization layer design adaptations, biopolymer and nanomaterial involvement and functional component cooperativity are themes of current projects.



## SERS-based biosensors for medical applications

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### Abstract

Surface enhanced Raman scattering (SERS)-based biosensors have drawn much attention in biomedical fields owing to their highly sensitive, non-destructive, and multiplexing capability. The key to realizing SERS potential in bioanalysis depends on strong electromagnetic enhancement of plasmonic materials and probe-target interactions for the trace detection of biomolecules regarding disease diagnostics, and monitoring. Gold nanorods (AuNRs) have been utilized in SERS-based biosensors for the detection of biomolecules such as cells, proteins, and oligonucleotides, due to their strong light absorption and scattering. In this presentation, we demonstrate the fabrication of SERS tags consisting of AuNRs conjugated with Raman reporters and targeting ligands for three biomarkers analysis. First, SERS tags consisting of Raman reporters and aptamer specific to target cells attached on AuNRs surface are applied for cervical cancer detection with high selectivity. Second, the determination of miR-29a, a biomarker of cancers, using SERS tags and magnetic separation is described with high selectivity and sensitivity in picomolar range. Lastly, SERS tags are constructed for the analysis of glycated human serum albumin (GHSA), a protein biomarker of diabetes mellitus (DM), with limit of detection nanogram range. These suggest the significant capability, feasibility, and versatility of SERS-based biosensors for sensitive and selective target analysis in medical applications.

*Keywords: Surface enhanced Raman scattering (SERS), gold nanorod, biomarker, cancer, diabetes mellitus*



**Short Bio: Suwussa Bamrungsap, Ph.D.**

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**Employment**

2011-Present      Researcher at Nanodiagnostics device (NDx) research team, Responsive material and nanosensors (RMNS), National Nanotechnology Center, Thailand

**Scholarship Awards and Honors:**

2020              L'Oréal Thailand's 'For Women in Science 2020' in Life Science  
2018              DMSc medical research award from Department of Medical Sciences, Ministry of public health  
2017              Poster award in The 1st MRS Thailand Conference, 2017, Chiang Mai  
2017              Supporting grant for new researchers, Thailand Research Fund (TRF)  
2016              Dissertation award from The National Research Council of Thailand (NRCT)  
2014              Research grants under H-GUARDS project, South Korea  
2012              Research Funding for DPST Graduate with First Placement  
2012              Poster award in Nanobiotechnology, IUMRS-ICYRAM 2012, Singapore  
2011              Graduate Student Travel Funds, University of Florida, USA  
2006-2011      Scholarship from National Nanotechnology Center, Thailand, The

**Royal Thai Government, Thailand**

1995-2006      Scholarship from the Development and Promotion of Science and Technology Talent Projects (DPST), The Royal Thai Government, Thailand

**Education**

2006-2011      Ph.D. (Physical Chemistry), University of Florida, FL, USA  
2003-2006      M.Sc. (Physical Chemistry), Kasetsart University, Thailand  
1999-2003      B.Sc. (Chemistry, Honors), Kasetsart University, Thailand

# Modelling the Aggregation of Mirna Cancer Biomarkers on a Graphene Quantum Dot

Tadsanee Awang<sup>a</sup>, Darunee Triphoton<sup>a</sup>, Nattapon Kuntip<sup>c</sup>, Deanpen Japrun<sup>b</sup>  
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## Abstract

MicroRNAs (miRNAs) are small non-coding RNA molecules associated with the regulation of gene expression in organisms. MiRNAs act as potential cancer biomarkers due to their involvement in the cancer development. Many attempts have been made to detect miRNA biomarkers, there is a lack of effective extraction strategies. Recently, graphene quantum dots (GQDs) contribute to several disease biosensor platforms including miRNA detection, but no application for miRNA extraction is investigated. A nanosized GQD seems to be suitable for small miRNA molecules where the miRNA adsorption and desorption on GQD are the key. The goal is to explore the possibility of using GQD for miRNA extraction. Thus, in this work, the assembly mechanism of miRNAs on GQD in solution is explored using Molecular dynamics (MD) simulations. The assemblies of pure and mixture of miRNAs (miR-29a and miR-144) on GQD(s) were studied. The results display the simultaneous assembly of miRNA-GQD complex. Our finding highlights the ability of GQD in collecting miRNAs in solution. Multiple miRNA conformations are captured. Interestingly, GQD shows miRNA selectivity. The effect of adding complementary DNA is also studied here. An insight obtained here can be useful for developing miRNA extraction and detection methods.

**Short Bio: Prapasiri Pongprayoon (Assoc Prof)**

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**Education**

- 2000-2004      **Bachelor of Science in Chemistry**  
Supervisor: Assist. Prof. Nojaree Prasipan  
Project title: *Extraction of natural products from rattan shoots found in Thailand*  
Kasetsart University, Thailand
- 2004-2006      **Master of Science in Physical Chemistry**  
Supervisor: Assoc. Prof. Supa Hannongbua  
Thesis title: *Particular interactions of MLN-4706 with Angiotensin-converting enzyme 2 using quantum calculations*  
Kasetsart University, Thailand
- 2005-2006      **Master of Research in Bioinformatics** (with Distinction)  
Supervisor: Dr. Emanuele Paci  
Thesis title: *Statistical correlation between structure and function of cold shock proteins*  
University of Leeds, UK
- 2006-2010      **DPhil in Biochemistry**  
Supervisor: Prof. Mark SP Sansom  
Thesis title: *Molecular modeling of  $\beta$ -barrel outer membrane proteins*  
Wolfson college, University of Oxford, UK

**Awards, Fellowships, Grants**

- 1998-2000      The King Bhumibol's Awards for the group of Rajchavinit schools  
2000              Second prize's winner of 180 IQ TV program (Grade 12)
- 2001-2004      Scholarship from the Charoen Pokphand Group of companies  
(undergraduate)
- 2004-2005      The Postgraduate scholarships on Education and research in Petroleum  
and Petrochemical Technology (Master degree in Physical chemistry)
- 2005-2010      Higher Educational Strategic Scholarships for Frontier Research network (Master-DPhil)
- Sep 2011        Epson travel grant from ISTCP-VII conference
- Oct-Nov 2011   Junior research fellowships from the French government (2 months)  
*Topic:* Simulations studies of a leukotriene BLT2 GPCR receptor,  
*Mentor:* Dr Marc Baaden, Institut de Biologie Physico-Chimique, Paris, France
- Apr-Jun 2012   ASEA-Uninet research fellowships (2 months)  
*Topic:* Coarse-Grained simulations of voltage sensor from Na channel  
*Mentor:* Prof. Karl Peter Wolschann, University of Vienna, Austria
- Nov 2016-Jan 2017   IMS-IIPA (2 months)  
*Topic:* Investigating sugar binding affinity to human serum albumin  
*Mentor:* Prof. Shinji Saito, Institute of Molecular Science, Japan
- July 2017-Jan 2018   Endeavour research fellowships (6 months)  
*Topic:* Investigating sugar binding affinity to human serum albumin  
*Mentor:* Assoc. Prof. Ben Corry, Australian National University,  
Australia

# Plasmonic Nanowire SERS Endoscopy for Unveiling Intracellular Drug Dynamics

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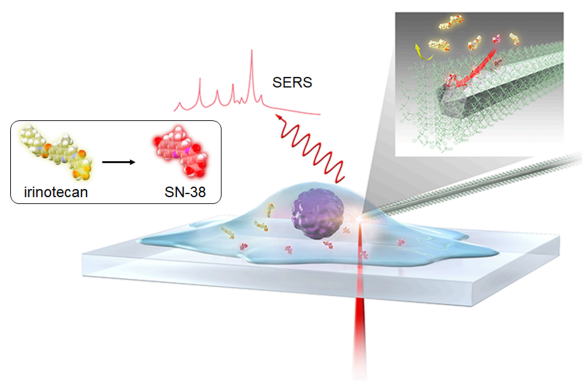
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## Abstract

Understanding the dynamics and distribution of medicinal drugs in living cells is essential for the design and discovery of treatments. Nonetheless, the tools available for revealing this information are extremely limited. Recently, our group has introduced the utilization of plasmonic silver nanowires (AgNWs) as novel Surface-enhanced Raman scattering (SERS) endoscopic probes for detecting signals within cells at desired locations. This method of AgNWs-guided SERS endoscopy offers unique spatiotemporal resolution: the probe is inserted into a specific region of the living cell using a 4-axis micromanipulator, and then, the laser is focused at the tip of the nanowire probe (direct excitation) where SERS signals from the intracellular environment are collected. While the direct excitation configuration generated a limited SERS enhancement, the application of remote excitation, by separating the point of focused laser excitation from the point of detection, enabled the acquisition of SERS spectra with a lower background, higher signal-to-noise ratio, and minimal associated photodamage. Importantly, it is demonstrated that the probe insertion does not induce stress to the cell. The high sensitivity and fingerprinting capabilities of this method allow the observation of non-fluorescent molecules, identification of their structural conformation and molecular interactions, and even monitoring the dynamic changes. In this presentation, we report the application of SERS endoscopy and probe design to monitor the intracellular fate and dynamics of drug molecules in cancer cells.



**Figure 1.** Schematic illustration of selective detection of MOF-coated nanowire probe inside cells. SN-38 (red) is selectively adsorbed by the MOF coating, instead of irinotecan (yellow) and biomolecules (blue), and diffuses to the surface of the silver nanowire, where SERS signals of SN-38 are detected, providing information on intracellular hydrolysis of irinotecan and localization of SN-38.

**Keywords:** Single-cell endoscopy, SERS, Silver nanowire

# Antibody-Aptamer SERS-based Lateral Flow Immunoassay (SERS-LFIA) for The Quantitative Detection of Human Serum Albumin Protein

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## Abstract

Albumin is the most abundant protein in blood plasma that plays crucial roles in maintaining blood osmotic pressure and transporting hormones, enzymes, minerals, and drugs. A normal range of human serum albumin is 3.5 – 5.5 g/dL. A decreased albumin level (hypoalbuminemia) may serve as indicative markers for conditions such as hepatic and renal disorders, malnutrition, or inflammatory diseases. The quantification of albumin level is conventionally done as part of a routine blood test within hospital or large medical laboratory settings. Herein, we report a novel platform as a proof-of-concept for the quantitative, rapid, and simple detection of human serum albumin protein, with potential for use in point-of-care (POC) settings. This was achieved by utilising an aptamer and an antibody specific to the human serum albumin protein as recognition molecules and gold nanoparticles (AuNPs) labelled with malachite green isothiocyanate (MGITC) for a surface-enhanced Raman scattering-based lateral flow immunoassay (SERS-LFIA). The proposed platform facilitated rapid qualitative detection through naked eye within 30 minutes. Subsequently, the quantitative analysis was achieved using a portable Raman spectrometer to map the SERS signal across the test spot. The dynamic range of our proposed platform for human serum albumin protein detection spanned from 0.25 – 4 g/dL, thereby enabling the assessment of the decrease in human serum albumin level associated with health concerns. The use of the portable Raman spectrometer, in place of a commonly used benchtop Raman spectrometer, presents substantial potential of our proposed platform for the quantitative, rapid, simple, and cost-effective detection of human serum albumin protein within POC settings.

*Keywords: Antibody, Aptamer, Surface-enhanced Raman Scattering (SERS), Lateral Flow Immunoassay (LFIA)*

# Hepatoprotective Effect of Zinc Oxide Nanoparticles Against Non-Alcoholic Fatty Liver Disease in Hepatocellular Carcinoma Cells

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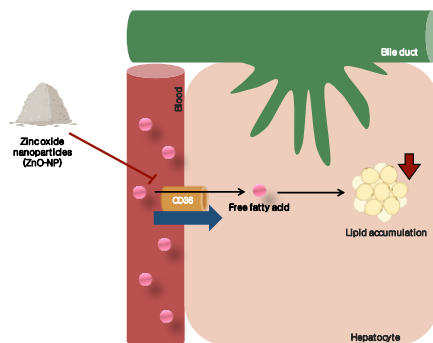
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## Abstract

Non-alcoholic fatty liver disease (NAFLD) is characterized as the most common hepatic manifestation affecting a significant number of individuals worldwide. The onset of immoderate hepatic lipid accumulation is primarily attributed to the free fatty acid (FFA) influx, rendered by cluster of differentiation 36 (CD36). Therefore, mitigating CD36 could potentially ameliorate the NAFLD condition. In which, zinc oxide nanoparticles (ZnO-NP) have recently drawn significant global attention regarding to their diverse biomedical applications, including anti-inflammatory, antioxidant, and antidiabetic properties. However, a common issue with commercially available ZnO-NP is their tendency to assemble and cause agglomeration. Herein, ZnO-NP derived from flame spray pyrolysis synthetic methods is being provided to outperform the commercially available, especially in the context of NAFLD prevention. The human hepatocellular carcinoma (HepG2) cells were co-incubated with free fatty acids either in the presence of ZnO-NP or commercial ZnO-NP. Following that, intracellular lipid content as well as CD36 expression level were evaluated through fluorescence staining using flow cytometry and quantitative real-time PCR, respectively. Results show that ZnO-NP exhibited hepatic lipid-lowering effects by decreasing lipid content together with downregulating CD36 mRNA expression superior to commercial ZnO-NP without interfering cell viability. Taken together, ZnO-NP offers a unique platform for lowering hepatic lipid accumulation over commercial ZnO-NP, partially through decreased hepatic FFA uptake. However, it is necessary to conduct further investigations to explore the precise targeting of ZnO-NP. In which, it could potentially be developed as a well-designed personal medicine to prevent individuals from developing NAFLD and related complications.

**Keywords:** Zinc oxide nanoparticles, Lipid-lowering effect, Hepatic steatosis, NAFLD, CD36

## Graphical abstract



## Zinc oxide nanoparticle from Flame spray pyrolysis (FSP ZnO-NP) alleviate intestinal cholesterol absorption in intestinal Caco-2 cells

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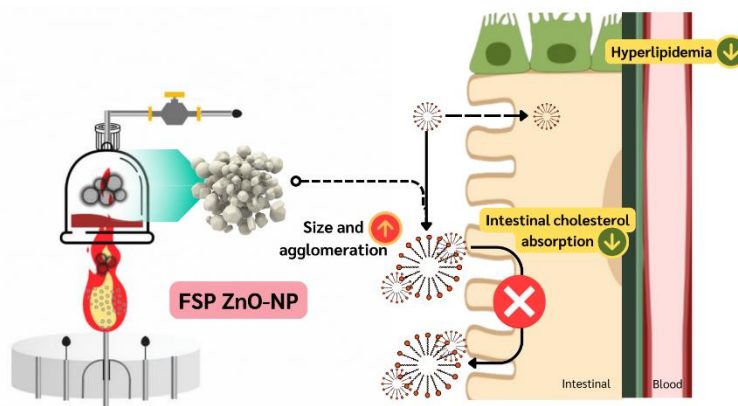
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### Abstract

Nanotechnology has been intense attention in various fields, such as, food industry and biomedical sciences owing to its outstanding properties. Among these, Zinc oxide nanoparticle (ZnO-NP) are the most abundantly used in the treatment and prevention of human diseases. At the present, ZnO-NP derived from flame spray pyrolysis (FSP ZnO-NP) firstly exhibits the advantage over other commercial ZnO-NP (c ZnO-NP) due to it is a one-step synthesis process with high purity, high external surface area, high noble metal dispersion, and could be produced in a large scale. However, the potential benefit in biomedical field is limited. Thus, this study determined the lipid-lowering activities of FSP ZnO-NP using in vitro and intestinal Caco-2 cells. FSP ZnO-NP was co-incubated with cholesterol micelles and subsequently determined physicochemical property of the micelle cholesterol. The 3-dimensional structures of micelle cholesterol after exposure to FSP ZnO-NP was also identified using scanning electron microscope (SEM). Lipid-lowering effects of FSP ZnO-NP was investigated by the fluorescent-cholesterol micelles absorption in the intestinal Caco-2 cells and cell viability was also confirmed. Results showed that both FSP ZnO-NP and commercial ZnO-NP (c ZnO-NP) were not effect to the micellar cholesterol solubility. However, FSP ZnO-NP increased cholesterol micelles size together with agglomeration more than c ZnO-NP. Correspondingly, the rate of fluorescent-cholesterol absorption was markedly decreased by FSP ZnO-NP when compared with control cells and c ZnO-NP without any cytotoxicity. This findings suggest that FSP ZnO-NP exhibits lipid-lowering effect by inhibiting intestinal cholesterol absorption, partly, by increasing cholesterol micelle size and agglomeration. Thus, ZnO-NP could potentially be developed as novel agent for preventing hyperlipidemia. However, further investigation is crucial needed to illustrate the precise mechanisms involved with FSP ZnO-NP's effects as well as its safety use in humans.

**Keywords:** Zinc oxide nanoparticle, Flame spray pyrolysis, cholesterol absorption, cholesterol micelles, lipid-lowering effects



## Effect of the Ethanol-to-Water Ratio on The Properties of Silica–Carbon Core–Shell Materials for Prolonged Antibacterial Activity of Thymol

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### Abstract

Porous silica (SiO<sub>2</sub>) nanoparticles have been widely used as drug-delivery materials; however, it is difficult to control drug release at desirable rates when using only SiO<sub>2</sub>. Thus, a facile synthesis of SiO<sub>2</sub>-carbon core-shell (SiO<sub>2</sub>@C) nanoparticles with tunable sizes and shapes for efficient controlled release was developed to prolong the antibacterial activity of thymol (T). The physicochemical properties, and surface bonding between thymol and the carbon shell were determined with XPS, NEXAFS, and DFT studies. An *in vitro* thymol release study was also applied, and the prolonged antibacterial performance was evaluated with gram-positive *Staphylococcus aureus*. The optimal conditions for producing spherical SiO<sub>2</sub>@C core-shell nanostructures with a uniform size distribution included an ethanol-to-water ratio of 20:80 (E20W80). This produced a SiO<sub>2</sub>@C core-shell material with a high porous carbon content and a large pore volume. Moreover, SiO<sub>2</sub>@C-T exhibited the highest thymol release profile. DFT studies demonstrated that the thymol was physically adsorbed on the carbon surface. This adsorption mode was advantageous for prolonged release. Consequently, the bacteriostatic agent SiO<sub>2</sub>@C-T E20W80 showed sustained thymol release levels of up to 40% over 48 h. The developed SiO<sub>2</sub>@C material shows potential for use as a nanocarrier of drug/active ingredients.

**Keywords:** SiO<sub>2</sub>@C core-shell, Nanocarrier, Thymol, Antibacterial activity, Slow release



# Screen-Printed Graphene Electrodes for 11-Nor-Delta-9-Tetrahydrocannabinol-Carboxylic Acid Based on Electrochemical Sensing.

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## Abstract

For centuries, further breakthroughs in nanomaterials for screen-printing techniques show several advantages in the areas of electrochemical sensor. Several research have been developed these techniques to fabricate high-performance electrodes. This research proposes a method development of an electrochemical sensor for selective and sensitive monitoring of narcotic, 11-nor-delta-9- tetrahydrocannabinol-carboxylic acid (THC-COOH), using disposable screen-printed graphene electrodes (SPGEs). For electrodes fabrication processes, the graphene ink was prepared by mixing 5 wt. % of graphene powder with carbon paste (CP) using a ball milling machine. The ink was then screened on polyethylene terephthalate (PET) substrates as working electrodes (WE) and counter electrodes (CE). Then, a silver-silver chloride paste (Ag/AgCl) was screened as reference electrode (RE), followed by insulating paste as insulator. A small sample volume of only 50 microliters was required for the detection of disposable SPGEs by the developed-electrochemical analyzer. The developed electrode was then applied for the THC-COOH by using square wave voltammetry (SWV). Optimal condition of SWV obtained at start voltage -0.20 V stop voltage 0.30 V, 20 mV step potential, 100 mV amplitude, 1 Hz frequency. The narcotic sensing system showed a wide analytical range of 50 to 1,000 ng/mL and low detection limit (LOD) of 32.79 ng/mL, that is detectable for cut-off values at 50 ng/mL. Thus, the proposed disposable SPGEs is an effective method for narcotic detection.

**Keywords:** Graphene, Screen printed-graphene electrodes (SPGEs), Electrochemical technique, 11-nor-delta-9-tetrahydrocannabinol-carboxylic acid (THC-COOH), Narcotic

# Nanoporous Composites for Environment, Catalysis, and Medicine

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## Abstract

Nanoporous materials comprise a relatively wide class of systems, usually divided in microporous (below 2 nm), mesoporous (between 2 and 50 nm) and macroporous (above 50 nm) materials. The porosity in materials, among all, is relevant in three great areas: environment, catalysis, and medicine. Indeed, nanoporous materials can act as collector of a wide range of organic and inorganic noxious species that contaminates soil and water. Porous substrates are fundamental in increasing the surface area and therefore the contact with reactants in catalysis. Also, porous particles can act as reservoir of therapeutic compounds in drug delivery.

Among the above-mentioned classes, microporous materials represent an area of increased popularity, as several small molecules fit into a 2 nm space. In the past decade the so-called porous coordination polymers (PCPs), popularly known as Metal-Organic Frameworks, or MOFs, have represented the most exciting class of porous materials thanks to their superior surface area (more than 1000 m<sup>2</sup>/g), tunable porosity, extreme synthetic flexibility thanks to the choice between inorganic nodes and organic linkers, and, most importantly, the ability to accommodate guests, also bigger than their pore size, thanks to a mechanism of self-assembly.<sup>(1)</sup> This aspect provides an enormous opportunity to make composites with unprecedented properties, arising from the pore selectivity of MOFs and the additional functionality of the guest species. Several materials can be embedded into the porous cage, from inorganic nanoparticles<sup>(2,3)</sup> to biomolecules.<sup>(4,5,6)</sup>

MOFs have been used in environmental remediation,<sup>(7)</sup> for example in the detoxification of water from hazardous transition metals,<sup>(8)</sup> as scaffolds for the preparation of advanced and recoverable metal<sup>(9)</sup> and bio-catalysts,<sup>(10)</sup> and as platform for drug delivery,<sup>(11,12)</sup> gene transfection,<sup>(13)</sup> therapeutics storage,<sup>(14)</sup> and antibody-based sensing.<sup>(15)</sup> In this communication, the most innovative solutions regarding applications of nanoporous composites based on MOFs are presented, with a perspective vision of the future directions of this exciting discipline that is still developing its full potential.

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**Keywords:** Metal-Organic Frameworks, Porous Materials, Environment, Catalysis, Medicine

# Synthesis of *Chlorophytum borivillianum* mediated synthesized silver nanoparticles and their antioxidant and antibacterial activities

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## Abstract

### Background:

The unexpected onset along with the rapid spread of infections caused by bacteria, in addition to the regular development of resistance to typical molecular drugs, emphasize the urgent requirement for alternative methods to kill or inactivate infectious pathogens. Green silver nanoparticles generated using plant extracts demonstrate resilient antimicrobial properties, as a result of recent advances in nanotechnology.

### Methodology

The synthesis of silver nanoparticles was carried out in this study by employing the aqueous root extract of *Chlorophytum borivillianum*, along with a reducing solution containing 1 mM silver nitrate (AgNO<sub>3</sub>) and microwave irradiation. The silver nanoparticles synthesized through green methods were characterized using various techniques, such as UV-Vis's spectroscopy, Energy dispersive X-ray spectroscopy (EDS), Fourier Infrared Spectroscopy (FT-IR), Transmission Electron Microscopy (TEM) and antioxidant activity. Antibacterial activity of green silver nanoparticles was carried out on *Staphylococcus aureus* and *Salmonella typhi*.

### Results:

Morphologically, the nanoparticles were pleomorphic in shape with a molecule size of 40-60 nm. The presence of potential biomolecules necessary for the reduction of silver ions is demonstrated by FT-IR spectral analysis of the extract as well as the nanoparticles. Silver nanoparticles synthesized with help of *Chlorophytum borivillianum* were found to be effective antioxidants. These green silver nanoparticles are effective in inhibiting the growth of multidrug resistant *Staphylococcus aureus* (MRSA), clinical isolate of *Salmonella typhi* with very high potential.

### Conclusion:

These findings demonstrate that *Chlorophytum borivillianum* root extract could be utilized as a mediator for synthesis of silver nanoparticles and have act as potent antimicrobial and antioxidant agents.

# Mesoporous Silica Nanoparticles Conjugated with Curcumin as a Redox-Responsive and Targeted Drug Delivery Agent for Brain Cancer Therapy

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## Abstract

The blood-brain barrier (BBB) is a barrier to avoid unwanted molecules from the blood circulation to enter the central nervous system. This feature introduces difficulties in treating brain cancer patients. The ability of nanoparticle drug carriers to cross the BBB is very important for brain cancer therapy besides common properties such as low toxicity, good stability, and targeted and controlled drug release to cancer cells. In this study, the drug was conjugated to MSN via a disulfide bond of 3,3'-dithiodipropionic acid (DTDP), which is responsive to redox stimuli (MSN-SS-D). MSN-SS-D was then modified by the addition of Tet-1 peptide (MSN-SS-D/Tet-1) on the surface to make it able to cross the BBB. Drug conjugation with DTDP was confirmed by nuclear magnetic resonance (NMR) analysis. MSN-SS-D/Tet-1 was confirmed by analysis of Fourier transform infrared spectroscopy (FTIR), dynamic light scattering (DLS), zeta-potential, thermogravimetric analysis (TGA), and transmission electron microscope (TEM). A drug release test was carried out at pH 4.8 and 7.4 with PBS solution added with glutathione (GSH) as a redox trigger for disulfide bonds. This shows that the release of drugs conjugated with linker disulfide can increase their effectiveness. These results indicate that this drug delivery system can be an effective strategy for brain cancer therapy.

*Keywords: Tet-1, redox-responsive, silica nanoparticle, drug delivery, brain cancer*

# Hydrothermal Optimization of Bicontinuous Concentric Lamellar (bcl) Mesoporous Silica for Enhanced Drug Loading

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## Abstract

Mesoporous silica (MS) is one of the most promising materials as a drug carrier in cancer treatment because of its good properties. Bicontinuous Concentric Lamellar Mesoporous Silica (BMSN) is a silica-based material with a flat structure arranged radially in a three-dimensional (3D) open channel structure. One of the important requirements for its use as a drug carrier is the BMSN's ability to load drugs well. The most influential thing in drug loading is the size and pore diameter of the material. Pore formation using the hydrothermal method is strongly influenced by temperature, reaction time, and the molar ratio of the reagent itself. For this reason, silica hydrothermal optimization was carried out here to achieve a material with maximum drug loading. The results obtained were characterized by surface area analyzer, SEM, FTIR, and drug loading studies. In the FTIR results obtained, the successful synthesis of BMSN can be shown by the presence of vibration absorption in the area of  $\sim 850\text{ cm}^{-1}$  which indicates the presence of the Si–O functional group, and at the wave number of  $\sim 1200\text{ cm}^{-1}$  indicating the presence of the Si–O–Si functional group. The wave number  $2900\text{--}3000\text{ cm}^{-1}$  shows vibration absorption from C–C, this is because there is still a surfactant template in the form of CTAB. The surface area analyzer results show results in the 2–50nm range which indicates mesoporous material.

*Keywords: drug carrier, cancer, bicontinuous concentric lamellar mesoporous silica, hydrothermal method*

## Methanethiol electroanalysis with carbon nanotube/gelatin-modified glassy carbon electrodes

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### Abstract

Reported is the amperometric anodic detection of methanethiol ( $\text{CH}_3\text{SH}$ ) at disk-shaped glassy carbon electrodes (GCEs) that carried thin films of a carbon nanotube/gelatin (CNT/G) composite as a functional surface modification. Placement of the nanofibrous/nanoporous CNT layer had the task to enlarge the active sensing area and reaching electrochemical signal amplification while the topcoat of gelatin glued the CNT cover to the smooth GCE surface and protected against otherwise likely CNT film delamination. CNT/G-GCE sensor preparation involved the sequential execution of two simple drop & dry steps, first with a homogeneous suspension of CNT in water and then with a diluted gelatin solution. For  $\text{CH}_3\text{SH}$  measurements completed sensor items were operated in a three-electrode electrochemical cell in amperometry mode, with a constant detection potential of + 0.12 V vs. Ag/AgCl/3 M KCl. Calibration trials verified a  $\text{CH}_3\text{SH}$  response linearity from 25 to 1,200  $\mu\text{M}$  and the practical limit of detection (LOD) for the analyte was identified as 5  $\mu\text{M}$ . Applications of CNT/G-GCE sensors for the determination of 50  $\mu\text{M}$  of  $\text{CH}_3\text{SH}$  in phosphate buffer model samples were successful with an adequate analyte recovery rate of  $98 \pm 5\%$ . As their fabrication is simple and cheap and as their performance is very good, the proposed  $\text{CH}_3\text{SH}$  sensors are recommended as sustainable tools for the electrochemical quantification of the compound in, for instance, environmental or biological samples. Own future work will target the use of CNT/G-GCEs for the indirect detection of methionine gamma-lyase, an enzyme that degrades sulfur-containing amino acids in body fluids to  $\alpha$ -keto acids, ammonia, and thiols and that has relevance as a clinical biomarker for diseases related to metabolic body dysfunctions.

*Keywords: Methanethiol, Carbon nanotubes, Amperometry, Gelatin*

## Chitosan Blending with Water-Soluble Polymers and Sugars as Dissolving Microneedles for Controlled Drug Release

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### Abstract

Chitosan microneedles have attracted significant interest in the field of transdermal drug delivery. This is due to their potential for painless and controlled drug administration. In this study, chitosan microneedles were prepared by incorporating polyvinylpyrrolidone (PVP) and polyvinyl alcohol (PVA) in three different ratios (1:1, 2:1, and 3:1 chitosan: polymers) to control drug release. The microneedles were fabricated using a molding method, their mechanical properties were tested using the universal testing machine (UTM), and their skin penetration ability was tested using pig skin (*ex vivo*). The results indicated that the microneedles exhibited sufficient strength to penetrate the outer layer of the pig skin effectively. The study included incorporating two drugs: curcumin as a model of hydrophobic drugs, and butterfly pea extract as a model of hydrophilic drugs. Maximum loading capacity was studied. Ability to send drugs into the skin was also proven.

*Keywords: Chitosan, Dissolvable microneedles, sustained release*

# Development of Novel Chemistry for The Fabrication of GFET

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## Abstract

Recently, the importance of the development for on-site rapid diagnosis technology is arising. Under the consecutive pandemic situation, the prevention of the infection of highly contagious pathogen is major concern. For the construction of universally applicable diagnosis platforms, there are few essential requirements such as (i) interfacing chemistry for the integration of conducting nanomaterials and receptors, (ii) production of stable form of bioreceptor, and (iii) cost-effective miniaturized handheld device. The introducing organic interfacial compounds (OICs; oligo(phenylene ethynylene)amine, N-heterocyclic carbene) improved the immobilization efficiency of bioprobe owing to forming by self-assembly monolayer on graphene. The receptor was embedded into lipid bilayer for the construction of the formulation for nanodisc that is highly stable under the existence of various biomaterials. The reversible reactivity of bioreceptor was presented and miniaturized sensor chip showed cost-effectiveness of our newly invented biosensor. Based on those primary technologies, our research proposed novel PoCT diagnosis platform integrating various nanobiotechnologies such as nanodisc immobilized GFET and ultra-fast photonic PCR. In a wide range of industries, such devices can be applied including food, electronics, and healthcare.

*Keywords: Nanobiosensor, Graphene Field-effect Transistor, Photonic PCR, Nanomaterials, Bioreceptor*



## SERS- based Biosensor for the Detection of Cortisol in Sweat

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### Abstract

Biosensors are getting increasingly attractive in the fields of early disease detection and health monitoring because of their potential for sensitive and selective detection of biomarkers in body fluids. Biomarkers improve our understanding of the human body by allowing us to track the development and course of ailments. Sweat is a body fluid containing various such possible indicators and offers a special source for continuous health assessment. It contains one of the useful biomarkers called ‘cortisol,’ which is accepted as a key biomarker for tracking the physiological stress brought on by infections or other daily habits. This research reports the prospective use of biosensing technique combined with another powerful technique known as surface-enhanced Raman scattering (SERS) for the detection of cortisol biomarkers in sweat. Plasmonic nanostructure integration in SERS substrates produces localized electromagnetic (EM) field enhancement for the Raman signal allowing sensitive detection. Rhodamine 6G (R6G) was used as an analyte for SERS substrate detection with 633nm excitation wavelengths. This substrate is good in Homogeneity structure with RSD =2.70%. The stability test prepared samples from fresh to 28 days is a 19.45% reduced signal intensity. The lowest R6G concentration detected from Confocal Raman spectroscopy is 10<sup>-9</sup>M, and the LOD = 90pM, with good reproducibility. For the purpose of detecting cortisol, a competitive immunoassay biosensor stage was used to monitor cortisol in sweat. Based on the results, the SERS-based competitive immunoassay exhibited great potential for high sensitivity and reliable detection of cortisol. SERS active gold (Au) nanoparticles tagged with a Raman reporter (4-MBA) was used as SERS tag in the competitive assay and using the biosensor cortisol concentrations as low as 10<sup>-9</sup>g/L was successfully detected in a synthetic sweat sample. The developed SERS-based biosensor showed excellent reproducibility, repeatability, selectivity, and stability at low analyte concentrations, making it a promising technique for monitoring physiological stress in human.

**Keywords:** Biosensor, Nanobiosensor, Surface Enhance Raman Scattering (SERS), Cortisol, Stress, Competitive immunoassay

# Upconversion Nanoparticles for Near-Infrared Photodynamic Therapy of Cancer

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## Abstract

Upconversion nanoparticles (UCNPs) that emit high-energy photons upon excitation by the low-energy near-infrared (NIR) light are emerging as new optical nano-probes useful in biomedicine. Herein, we load C-phycocyanin (CPC), a photosensitizer, on polymer-coated UCNPs, forming a UCNP-CPC complex that produces singlet oxygen to kill cancer cells under NIR light. This work designed polymer-coated nanoparticles based on UCNPs to trigger cancer immunotherapy by NIR-induced photodynamic therapy (PDT). The successful preparation of UCNP-CPC was confirmed via Transmission electron microscopy (TEM), X-ray diffraction (XRD), UV-visible spectroscopy, and Fluorescence spectroscopy. According to the results, UCNP-CPC is positively charged (27.4 mV) and has an average particle size of ~350 nm using dynamic light scattering (DLS), indicating the good stability of the UCNP-CPC complex. The UV-vis spectra of CPC absorption at approximately 621 nm and UCNP emission at ~620 nm to activated CPC by PDT. Under 980 nm laser irradiation, CPC is activated to destroy the cancer cell for deep tumors treatment. Thus, C-phycocyanin is a non-toxic fluorescent pigment that can be used in low-level light therapy.

*Keywords: laser therapy, nanomedicine, photodynamic therapy, upconversion*

## Graphene Oxide-Based Aptasensor for Sensitive Urinary Albumin Detection: A Clinical and Community Study

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### Abstract

In this study, we introduce a novel aptasensor designed for enhanced detection of urinary albumin, suitable for both clinical and point-of-care applications. The sensor employs a short, single-stranded DNA aptamer with high specificity for albumin, along with the fluorescence-quenching properties of graphene oxide (GO). This combination results in low limits of detection (LOD) and quantification (LOQ) of 50 ng·mL<sup>-1</sup> and 150 ng·mL<sup>-1</sup>, respectively, outperforming existing hospital methods. The detection mechanism involves forming a GO-aptamer complex, which initially exhibits a quenched fluorescent signal. When albumin is present, the fluorescent-labeled aptamer detaches from the GO and binds to the albumin, restoring the fluorescence signal in a concentration-dependent manner. The technology has achieved patent protection, received Thai FDA manufacturing authorization, and been featured in international journals. A field trial through the Chronic Kidney Disease Network (CKDNET) screened 84 urine samples, revealing that 12% had elevated albumin levels—primarily among those with diabetes or hypertension—and 50% indicated potential early signs of kidney dysfunction."

*Keywords: albuminuria, aptasensor, fluorescence quenching, portable fluorometer, chronic kidney disease*

## Minimally Invasive Glucose Monitoring with Molecularly Imprinted Polymer-Based Microneedle Biosensors

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### Abstract

Diabetes mellitus is typically diagnosed using invasive or enzymatic methods to measure blood glucose concentration, providing critical information about the patient's health. However, the accuracy of enzyme-based electrochemical glucose sensors is limited by strip manufacturing variances, improper storage, and aging. In this work, a microneedle (MN) molecularly imprinted polymer (MIP) approach has been used to develop an electrochemical non-enzymatic sensor to monitor glucose levels, facilitating a simple sampling fluid under the skin without bleeding. A cross-shaped microneedle patch was fabricated using a novel and convenient photolithography method. The microneedle patch was made from a non-cytotoxic bio-based resin derived from soybean oil and methyl methacrylic acid (AESO/MAA). The microneedle patch was then coated with gold nanoparticles using electroless plating and sputtering methods. Subsequently, the microneedle gold electrodes were deposited with MIP membrane using methacrylic acid (MAA) functional monomer and ethylene glycol dimethacrylate (EGDMA) crosslinker in the presence of a glucose template, processed through electropolymerization or spin coating. Cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and differential pulse voltammetry (DPV) techniques were utilized for the electrochemical measurements using potassium ferrocyanide as a redox probe in phosphate buffer saline. The microneedle MIP sensor effectively detected glucose within a range of 50 to 800 mg/dL, even at an elevated temperature of 50 °C before testing. This work demonstrates a simple and effective sensing platform that overcomes the limitations of microneedle electrode fabrication and enzyme-based strips, making it a promising tool for accurate and reliable non-invasive diagnosis in the future.

**Keywords:** Biosensor, Molecularly Imprinted Polymer, Electrochemistry, Glucose Sensor, Minimally Invasive, Diagnosis

## Electrochemical sensors for simultaneous sensing of multiple heavy metal ions based on gold nanostars modification on the screen-printed electrode surface.

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### Abstract

The purpose of the research described was to develop an electrochemical sensor with high sensitivity and selectivity for detecting heavy metal ions. The sensor was based on modifying a screen-printed electrode (SPE) surface with gold nanostars (AuNS). The modified electrode, referred to as AuNS/SPE, was investigated using Square Wave Voltammetry (SWV). This electrochemical setup proved to be highly effective in detecting heavy metal ions, specifically Cadmium, Lead, Copper, and Mercury, all at once. The AuNS/SPE exhibited excellent electrochemical sensing properties compared to a bare screen-printed electrode (Bare SPE). The sensor produced significant current signals at specific voltages for each heavy metal ion: -0.9 V for Cadmium, -0.55 V for Lead, -0.25 V for Copper, and 0.1 V for Mercury. This demonstrated the capability of the developed sensor to differentiate between these heavy metal ions based on their electrochemical behavior. The research findings suggest that this innovative electrochemical sensor has great potential for both quantitative and qualitative analysis of multiple heavy metal ions in water samples. Its application could be crucial in preventing and mitigating incidents of chronic kidney disease resulting from heavy metal ion contamination in drinking water. In summary, the research succeeded in developing an electrochemical sensor based on gold nanostars modified onto a screen-printed electrode. This sensor demonstrated high sensitivity, selectivity, and the capability to simultaneously detect multiple heavy metal ions in water samples. Given its potential benefits in preventing health issues related to heavy metal ion exposure, this technology could find practical applications in water quality monitoring and environmental protection.

*Keywords: Heavy metal, Electrochemical sensor, Square wave voltammetry, Screen printed carbon electrode, Nanomaterial, Chronic kidney disease*

## Electrochemical Biosensor for Detecting Aerobic Bacteria in Cow's Milk

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### Abstract

In this work, we proposed the electrochemical methods for the detection of total aerobic bacteria. Instead of using a biorecognition element, methylene blue is applied as a redox indicator to identify the presence of aerobic bacteria on a screen printed carbon electrode. The detection rationale is based on the measurement of different electrical potentials when the transformation of methylene blue occurs. At the presence of aerobic bacteria, they utilize oxygen in their intracellular metabolism, which leads to the conversion of methylene blue from its oxidized form to its reduced form. Consequently, the electrochemical signal changes are directly proportional to the number of bacteria growing. The operating conditions were optimized and established for sensing the electric current responses of *Escherichia coli* and *Staphylococcus aureus*. The sensing platforms provides a detection limit at 3 CFU/ml for both *Escherichia coli* and *Staphylococcus aureus* in UHT milk within 10 min at neutral pH. This technique offers the rapid and highly sensitive detection of aerobic bacteria, enabling improved efficiency of milk's quality analysis. Additionally, there is a potential for its further development into a portable device for on-site detection which will benefit for the improvement of cow's milk quality in both agricultural and industrial sectors of Thailand.

**Keywords:** aerobic bacteria, cow's milk, electrochemistry, biosensor

# Bifunctional Ternary Conjugated Pdots for simultaneous in situ Hydrogen Therapy and Fluorescence Imaging in NIR-II window

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## Abstract

In recent years, hydrogen therapy has shown great potential in clinical trials due to its anti-inflammatory and antioxidant activity. The primary methods of administration for Hydrogen in treatments include inhalation, drinking H<sub>2</sub>-rich water, and injecting H<sub>2</sub> saline. However, the limited solubility of Hydrogen in water and blood, as well as its high but aimless diffusibility, result in limited efficacy of the therapy in many diseases. [1] [2] In this study, we developed a novel ternary conjugated polymer dots (TCPdots) for in situ theranostics, which is the combination of hydrogen therapy and fluorescence imaging in second near-infrared window (NIR-II, 1000-1700nm). To achieve this, two types of dibenzothiophene (DBT)-core conjugated polymers with an ultra-low bandgap were developed as electron-acceptor materials, while PM6 and ITIC-based polymers were used as electron-donor materials to prepare TCPdots. By exploring the intermolecular interactions with different ratios of acceptor and donor materials and two types of ultra-low bandgap conjugated polymers, we aimed to create TCPdots with hydrogen evolution capability in the NIR-I window and emission capability in the NIR-II window. The series of TCPdots exhibited absorption at 650-900 nm and emission ranging from 950-1400 nm. Notably, the emission intensity of TCPdots at 1100 nm was twice that of Indocyanine green (ICG), which is usually used in NIR medical diagnostics, and this was achieved in just 0.3 seconds. Benefiting from the ultrahigh brightness and broad range of emission, we performed in vivo high-resolution angiography in mice using a 1300 nm long-pass filter. These bifunctional TCPdots can be applied to theranostics, enabling the simultaneous achievement of non-invasive, deep-tissue in vivo NIR-II imaging, and paving the way of in situ hydrogen therapy

*Keywords: conjugated polymer, hydrogen therapy, theranostics, near-infrared window*

## Multi-layer Silicene Nanosheets Derived from End-of-life Solar Cells for Use as Anodes in Lithium-ion Batteries

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### Abstract

Silicene, with its unique two-dimensional (2D) layered Si nanosheets, has been attracting increasing attention in recent years. This is due to its graphene-like structure and outstanding anode properties. There have been a few experimental studies of anodes in lithium-ion batteries (LIBs). The main problems are limited material resources and complicated production methods, which limit its practical applications. Therefore, large-scale and high-quality fabrication of silicene using green methods and sustainable material sources is currently an urgent challenge, especially for commercial applications. In this work, we fabricated a multi-layer silicene derived from end-of-life (EOL) silicon solar cells using chemical activation and exfoliation processes. Most synthesized silicene sheets are multi-layered with typical thicknesses between 1.73 to 3 nm. Then, it was employed as an anode material in LIBs. The silicene/graphite composite shows a stable reversible capacity of ~290 mAh g<sup>-1</sup> at a current density of 1C after 500 cycles. This anode had a Coulombic efficiency (CE) above 97% and greater than 93% capacity retention. Our composite material shows good integration in a single system, leading to improved capacity and enhanced stability. To the best of our knowledge, this is the first time that a recycling process for solar waste has been used to produce material for fabrication of multi-layer silicene that can be used as an anode material in LIBs. Furthermore, this work also provides a new opportunity in material recycling to produce silicene for fast-charging batteries, given an ever-growing number of EVs and for a more sustainable energy future.

*Keywords: silicene, two-dimensional, exfoliation, anode material, lithium-ion batteries*



# Toward High-Performance Zn ion Batteries

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## Abstract

Lithium-ion batteries (LIBs) have been widely studied and almost dominated the secondary battery market due to their higher energy density. Although the commercialization of LIBs has brought us great convenience, the availability and price of lithium (and cobalt) resources and the security risks stemmed from the flammable nature of organic electrolyte make them noncompetitive in large-scale applications. In recent years, the rechargeable aqueous zinc-ion batteries (ZIBs) are recognized as promising candidates for large-scale energy storage application in the post-LIBs era, because of the abundant reserves (75 parts per million in earth's crust), high theoretical capacity (819 mA h g<sup>-1</sup>) and low redox potential (-0.763 V vs. standard hydrogen electrode (SHE)) of zinc, as well as the non-flammable and high ion conductivity (1 S cm<sup>-1</sup>) of aqueous electrolyte. In a typical prototype, ZIBs consist of zinc metal anodes, (in)organic cathodes, neutral or slightly acidic aqueous electrolytes and separators. However, they are plagued by the lack of suitable cathode, electrolyte, separator, and the corrosion, hydrogen evolution reaction and dendrites growth in the Zn anode side, which limit their further development to meet commercial requirements. To be truly competitive with other rechargeable batteries, the efforts have been made toward the exploration of cathodes, anodes, electrolytes, and separators in recent years. Here, we present our strategies of improvement, including materials coupling [1], doping engineering [2,3], defect engineering [4] and novel cathodes in cathodes [5, 6], interfacial modification and zinc-free in anodes [7, 8], electrolyte additives [9, 10], and separator design [11-13], that enables the dendrite-free, high energy and power densities, long lifespan zinc ion batteries. Importantly, the gel polymer electrolytes were also applied for the pouch cell ZIBs during the practical application evaluation, which also displays a great deal of potential to fabricate flexible and wearable devices for future applications. Considering their distinctive merits of low-cost, environmentally benign, and high security, it is strongly believed that aqueous ZIBs possess enormous prospects and will be taken into application soon.

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**Research Area of Interest**

Batteries  
Supercapacitors  
Hybrid energy devices  
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2022	Editorial Board Member of Advanced Powder Materials
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2021	Associate Editor, Journal of Metals, Materials and Minerals (Scopus)
2018	Section Editor, Journal of Metals, Materials and Minerals (Scopus)
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2015	Editorial Board Member, Scientific Reports (Nature Publishing Group)
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## All-solid-state Supercapacitors Combining rGO and Dynamic Ion Gels

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### Abstract

Supercapacitors are energy storage systems that exploit electrochemical double-layer charge injection to deliver high energy storage densities and fast charge and discharge capacities. Optimal performance requires maximizing the interfacial area between the active materials and the electrolyte, as well as minimizing serial resistance without compromising mechanical stability. The need for lightweight, flexible, and safe devices is putting nowadays polymer-based materials in the spotlight. However, achieving the needed levels of safety (*e.g.* leakage of toxic liquid electrolyte and inflammation) and performance is still very challenging, especially since it requires an adequate combination of high-performance solid-state electrolytes with high-performance electrodes. Among promising candidates as both solid polymer electrolytes and ionic intercalation agents for stacked 2D materials (*i.e.* graphene), poly(ionic liquid)s (PILs), have received considerable attention at the conceptual level but they usually fail into providing the desired combination of ionic conductivity and mechanical properties.

Under the frame of our recent works, a new family of polyelectrolytes obtained via the complex coacervation of oppositely charged PILs or NPs building blocks, namely Dynamic Ion Gels (DIGs), has been developed. The gelation process is carried on via the creation of dynamic ionic crosslinks through ion metathesis with the concomitant in situ generation of ionic liquids (ILs). Such DIGs can be a potential candidate as a safe and quasi-solid-state electrolyte as well as ionic/polymeric intercalation agents for layered 2D materials, insuring highly conducting continuity through the whole device. Accordingly, combination with reduced graphene oxide (rGO) will lead to performing composites towards the development of all-solid-state supercapacitors. The elaboration of rGO/PIL or rGO/DIGs electrodes and their association with PIL or DIG electrolytes will be presented followed by storage performance evaluation at different operation conditions. Indeed, the fabricated cells can be efficiently operated at a high temperature (80°C) with a strong enhancement of performances compared to RT performances and without risk of liquid evaporation and leakage, which is not commonly obtainable with conventional electrolytes, even ionic liquids.

*Keywords: Supercapacitors, Solid-state Devices, Dynamic Ion Gels*

# 2D Materials: Bridging the Gap between Experiments and Data Mining for Cutting-edge Electrochemical Applications

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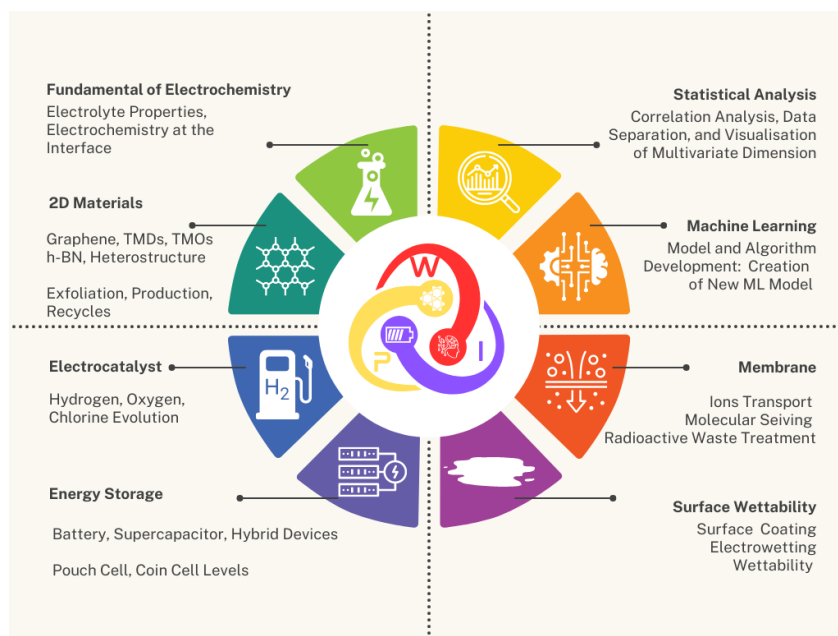
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## Abstract

Understanding the characteristics, both physical and electrochemical, of two-dimensional (2D) materials is crucial for the advancement of various electrochemical devices such as energy storage systems, electrocatalysts, ions selective membranes, and wastewater treatment technologies. To achieve this goal, controlled synthesis of 2D materials plays a vital role. In this study, we focus on the structural control achieved through liquid phase exfoliation of bulk materials, specifically: (i) **graphite-graphene**, (ii) **transition metal dichalcogenides**, and (iii) **heterostructure formation**. This involves material handling techniques and recycling of waste generated during the synthesis process. Furthermore, the exfoliated materials were utilised in diverse applications including supercapacitors (including electrode materials and binders), electrocatalysts, and removal of ions for wastewater treatment. To delve deeper into the complex realm of materials science and electrochemistry, we incorporated data science methodologies such as machine learning and statistical tools. Through simple data analysis, valuable electrochemical insights were derived, paving the way for the design of machine learning algorithms—an innovative approach in this field. To the best of our knowledge, this integration of data science as well as the materials synthesis in the context of 2D materials holds great potential for their development and application in various fields.



**Keywords:** 2D Materials, Electrochemistry, Data Science, Machine Learning, Applications

**Short Bio:**

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**Education**

Ph.D. Materials Chemistry  
University of Manchester, UK  
M.Eng. Chemical Engineering  
Kasetsart University, Thailand  
B.Eng. Chemical Engineering  
Kasetsart University, Thailand

**Awards**

Academic Excellent (Pure sciences), Anglo-Thai Society, United Kingdom, 2019  
Sheelagh Campbell Award, Royal Society of Chemistry, United Kingdom, 2019  
National Innovation Award, Research Council of Thailand, Thailand, 2017  
Royal Thai Government Scholarship, Ministry of Science and Technology, 2015

**Work Experiences:**

Jun 2023 to Present: Head of Research Unit  
Research Unit in Sustainable Electrochemical Intelligent, Thammasat University.  
Jul 2022 to Present: Faculty Member  
School of Bio-Chemical Engineering and Technology • Sirindhorn International Institute of Technology,  
Thammasat University.  
Jun 2021 to Jun 2022: Deputy Director  
(Research and Educational)  
• The Institute of Advance Materials and Energy Innovation  
• Rajamangala University of Technology Isan  
July 2020 to Jun 2022: Faculty Member  
Applied Physics • Rajamangala University of Technology Isan (RMUTI)

**Professional Activities**

Radioactive Waste Management Committee, Office of Atoms for Peace (Thailand), from 2023  
Guest Editor: Energies (Q1, IF 3.2524), MDPI (Switzerland)  
ISE member, ACS member, Reviewer in ACS, RSC, IOP, ISE, ECS journals  
Principal Investigator of 5 industrial grants (> 10M THB), and 5 Government/University funding.

**Research Area**

Electrochemistry: electrocatalyst, energy storage, electrowetting, potential-based membrane  
Two-dimensional Materials: Graphene, Transition metal dichalcogenides (MoS<sub>2</sub>, WSe<sub>2</sub>, MoSe<sub>2</sub>, and so on), Hexagonal boron nitrile, including the heterostructure forming.  
Large scale devices: Energy storage (Coin cell/Pouch cell), Ions and Molecular sieving membrane  
Machine Learning and Data Analysis: Neural networks, Decision tree based, Stacking in engineering.

# Materials graph neural networks and the discovery of solid-state electrolyte materials

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## Abstract

Finding novel solid-state electrolyte materials with specific desired properties is one of the main challenges of first principles-based modelling due to its high computational cost. Recently, machine learning (ML) has been used exclusively in the materials discovery field due to its remarkable capabilities to process large amounts of data and extract useful information insights.

By implementing materials graph neural networks, these networks were used to capture interatomic interactions and learn the underlying physics by representing molecules or materials as graphs. This approach reduces computational costs, enables the study of larger systems, and accurately reproduces structural energies and trajectories. It has the potential to accelerate materials discovery and facilitate the design of new materials with desired properties.

In this talk, we will discuss the basic theory and our recent work towards the development of ML model that can extensively discover and explore materials. We will highlight the computational-guided evolution approaches and screening high-performance Li conductor materials. Finally, we will end on discussing the future of ML-assisted materials discovery to the future of all-solid-state lithium batteries.

**Short Bio: Salatan Duangdangchote, Ph.D.**

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**Summary and Research Focuses**

My research primarily focused on accelerating materials discovery for advanced energy storage systems. As a Postdoctoral Fellow, I have specialized in solid-state electrolyte materials for Li-based batteries, utilizing state-of-the-art materials graph neural networks (GNNs) and machine learning techniques to analyze and predict material properties. Additionally, I have contributed to the development of a machine learning force field simulation suite and have a comprehensive understanding of material selection and structure design principles.

**Work Experience**

Postdoctoral Fellow 2022–Present

University of Toronto Scarborough, Scarborough, ON, Canada

Accelerating materials discovery primarily focusing on solid-state electrolyte materials for Li-based batteries

Extensive experience working with state-of-the-art materials graph neural networks (GNNs) e.g., CGCNN, MEGNet, SchNet, GemNet, SCN, DimeNet, PaiNN, etc.

Demonstrated expertise in utilizing GNNs and other machine learning techniques for analyzing and predicting material properties

Working knowledge of equivariant GNNs especially for molecular dynamics applications

Currently implementing new and modern ab initio molecular dynamics (AIMD) databases which will consist more than 250 million trajectories of ~2000 Lysuperionic conductors

Currently developing the integrating solution of machine learning force field simulation suite called GraNNField, which includes dataset generation tools, shared datasets across multiple GNN models, direct properties prediction, built-in molecular dynamics, and LAMMPS interface

Strong understanding of the material selection and structure design principles

Ability to conduct independent research or work effectively in a team environment, driving projects to successful conclusions



# A Heterogeneous Ionic Diode Membrane with High Geometry Gradient Based on Metal-Organic Frameworks for Efficient Osmotic Power Generation in Organic Solution

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## Abstract

Harvesting osmotic energy from organic waste solutions using an ion-selective membrane not only helps to alleviate environmental problems but also provides a clean and sustainable energy source. However, the development of highly selective and high-performance ion-selective membranes for these applications remains largely unexplored. Inspired by the electrocytes in electric eels which contain many angstrom-scale ion channels that allow preferential transport of ions in one direction, we have developed a metal-organic framework (MOF)-based heterogeneous membrane, which consists of HKUST-1 as the sub-nanoscale ion-selective layer and branched alumina nanochannel (BANM) as the supporting layer (known as HKUST-1@BANM), for efficient osmotic energy conversion from organic solutions. Due to the broken symmetries of charges and pore geometry, the HKUST-1@BANM shows strong ionic diode effect, that is, an amplified and directional ion transport, with a rectification ratio of up to 6.4 times in LiCl-methanol solution. Surprisingly, when tested under a 2 M feed solution mixed with pure methanol, the membrane generated electrical energy and achieved a power density of  $\sim 30.2 \text{ W/m}^2$ , which surpasses commercial benchmark ( $5 \text{ W/m}^2$ ). The increased power density can be attributed to the abundant and highly ordered channels that filter dehydrated cations and the membrane diode effect, which strengthens the ionic current that attracts cation transport through the membrane channels, leading to the generation of osmotic energy.

*Keywords: Salinity gradient power, Ion transport, Ion current rectification, MOF membrane, Nanofluidics*

## A New Electrokinetic Energy Generator Inspired by Trees

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### Abstract

Green clean energy has received great interest in recent years to tackle the increasing challenges caused by air pollution and excessive energy consumption. Despite rising awareness of clean energy production, the way to achieve high efficiency in energy conversion remains minimally explored. Inspired by the water transportation system in trees, we proposed a trapezoid-shaped (i.e., geometrically asymmetric) membrane with ionic rectification behavior for self-operating electrokinetic energy generation. The designed membrane is made of carbon black-coated hydrophilic filter paper, which can convert hydrostatic energy to electrical power with the supply of a few drops of water or salt solution on the tip (shorter base) side. Along the lateral direction of the trapezoidal membrane, directional ion transport could be initiated in nanofluidic systems with rapid water transport and evaporation. Compared to the symmetrical geometry (i.e., same width along the lateral/flow direction), the asymmetric membrane could create a typical ion current rectification (ICR), yielding a short-circuit current ( $I_{sc}$ ) of  $\sim 21 \mu A$  and an open-circuit voltage ( $V_{oc}$ ) of 0.5 V under ambient conditions (24 °C and 55% relative humidity). When connected in series and in parallel, the  $V_{oc}$  could maintain at a value of 1.75 V for over 10 days. In addition, the fabricated power generator with excellent flexibility could power LED bulbs of various colors and commercial calculator at room temperature. This pioneer research sheds light on the development of versatile energy conversion technologies from clean energy sources to supplement the increasing energy demand.

*Keywords: Electrokinetic power, Capillary flow, Transpiration, Electrical double layer, Water-enabled power generator,*

# Biomimetic Ionic Diode Membranes Based on Covalent-Organic Frameworks for Highly Efficient Energy Harvesting from Ionic Gradients

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## Abstract

Osmotic energy has emerged as an alternative candidate of sustainable energies due to the growing energy demand and the increasing awareness on environmental protection. An electric eel can produce high electrical energy when facing enemies that can even shock a crocodile by using sub-nanoscale biological channels in their cell membranes of electric organ to convert concentration chemical potential energy into electricity. Inspired by this, some researchers tried to do research in the field of osmotic energy conversion by fabricating an artificial membrane with nanoscale ion transport channels. Most of the previously reported membranes were based on nanoscale pores and disordered pore structures, leading to poor ion selectivity and insufficient ionic flux, and thus inferior power output. In this study, using the two-step interfacial polymerization, we for the first time report a two-layer covalent organic framework (COF) composite membrane (named as TFP-TPA/EB COF), which is composed of TFP-TPA COF and TFP-EB COF with opposite surface charge, for highly efficient energy harvesting from ionic gradients. Results obtained show that the TFP-TPA/EB COF membrane has sub-2 nm ordered straight ion channels and ionic diode property mimicking cell membrane channels. The TFP-TPA/EB COF can reach a record high power output under salt-lake water and river water. More importantly, we show that the prepared COF composite membrane can exhibit ultrahigh acid resistance, indicating its potential use in proton transport and energy harvesting from acid gradient. An amazingly high power density of  $\sim 170$  W/m<sup>2</sup> can be realized at a 100-fold proton gradient.

*Keywords:* Ion transport, Proton transport, Nanofluidics, Covalent-organic framework, Osmotic energy

# Sulfide Oxidation on Ladder-type Heteroarenes to Construct All-acceptor Copolymers for Visible-light-driven Hydrogen Evolution

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## Abstract

Conjugated polymers (CPs) have recently gained increasing attention as photocatalysts for sunlight-driven hydrogen evolution. However, they suffer from insufficient electron output sites and poor solubility in organic solvents, severely limiting their photocatalytic performance and applicability. Herein, solution-processable all-acceptor (A<sub>1</sub>-A<sub>2</sub>)-type CPs based on sulfide-oxidized ladder-type heteroarene were synthesized. A<sub>1</sub>-A<sub>2</sub>-type CPs showed upsurging efficiency improvements by two to three orders of magnitude, compared to their donor-acceptor (D-A)-type CP counterparts. Furthermore, by seawater splitting, PBDTTTSOS exhibited an apparent quantum yield of 18.9% to 14.8% at 500 to 550 nm. More importantly, PBDTTTSOS achieved an excellent hydrogen evolution rate of 35.7 mmol h<sup>-1</sup> g<sup>-1</sup> and 150.7 mmol h<sup>-1</sup> m<sup>-2</sup> in the thin-film state, which is among the highest efficiencies in thin film polymer photocatalysts to date. This work provides a novel strategy for designing polymer photocatalysts with high efficiency and broad applicability.

*Keywords: All-acceptor copolymer, sulfide-oxidized multifused ladder-type heteroarene, thin film, seawater splitting; photocatalytic hydrogen evolution*

# Nanoporous Activated Carbon from Rice Husk as Electrode Material: Enhancing Supercapacitor Electrochemical Performance

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## Abstract

Nanoporous activated carbon from rice husk was prepared via KOH activation at different ratios of rice husk: KOH, for using as electrode material in supercapacitor. The electrode could exhibit high performance in 6 M KOH aqueous electrolytes, particularly in terms of specific capacitance and power density. BET results indicated a high specific surface area of 1640.6 m<sup>2</sup>/g with a mesoporous type in a sample activated at a 1:3 ratio of rice husk:KOH. In this sample, a high specific capacitance of 195.36 F/g was obtained at a current density of 1 A/g with excellent cycles stability of 98.9% after continuous charge/discharge test for 10,000 cycles at 10 A/g. Moreover, the fabricated symmetric coin cell, in 6 M KOH aqueous electrolytes, could light up the LED bulb at 3V up to 900 seconds.

**Keywords:** Nanoporous activated carbon, Rice husk, Electrochemical performance, Electrode material, Supercapacitor

# Enhancing Nafion Electrolyte Membrane Performance with Zn-Based Metal-Organic Framework

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## Abstract

In this study, we investigated an application of metal organic frameworks (MOFs) as a proton conductors in electrolyte membrane. One-dimensional (1D) and two-dimensional (2D) Zn-based MOFs, incorporating the ligands imidazole ( $\text{ImH}_2^+$ ) and 1,2,4-triazole (TzH) respectively, were successfully synthesized by in situ method. Fourier-transform infrared spectroscopy results indicated that the N-H stretching vibrations in bulk TzH and  $\text{ImH}_2^+$  were responsible for a peak observed in both synthesized MOFs, centered at  $2500\text{--}3500\text{ cm}^{-1}$ . Thermogravimetric analysis profiles of the 1D and 2D Zn-based MOFs demonstrated thermal stability up to  $250\text{ }^\circ\text{C}$ , rendering them suitable for applications in moderately high-temperature environments. These MOFs exhibited an ion conductivity of  $1.29 \times 10^{-4}\text{ S cm}^{-1}$  at relative humidity. However, the incorporation of the metal-organic network material into Nafion led to enhancements in several properties of the composite membrane. In comparison to the pure Nafion membrane, the composite membrane demonstrated improved thermal stability up to 20 % and water molecule retention up to 30 %. Furthermore, the composite membrane displayed higher ion conductivity than the pure Nafion membrane. By increasing the ratio of metal-organic network components in the composite with the Nafion membrane, the performance of the Zn-based MOFs composite membrane surpassed that of the recast counterpart. However, an elevated ratio resulted in particle agglomeration, leading to reduced ionic conductivity. Despite this decrease, the ionic conductivity remained higher than that of the Nafion membrane. Significantly, the highest ion conductivity is  $1.52 \times 10^{-4}\text{ S cm}^{-1}$  at  $80\text{ }^\circ\text{C}$  and 95% relative humidity.

*Keywords: Zn-based MOFs, Composite membrane, Nafion membrane, Ion conductivity.*

## The effect of $\text{NiCo}_2\text{O}_4$ , $\text{NiCo}_2\text{S}_4$ , and $\text{NiCo}_2\text{Se}_4$ as Bifunctional Photoelectrocatalysts towards Zinc-air Batteries

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### Abstract

In recent years, zinc-air batteries have emerged as promising energy storage solutions, owing to their high specific capacity. However, a critical obstacle in their development is the slow kinetics of catalysts within the air-electrode component. This study focuses on investigating the catalytic performance of ternary nickel-cobalt chalcogenides, nanotubular  $\text{NiCo}_2\text{O}_4$ , as bifunctional photoelectrocatalysts for zinc-air batteries, emphasizing their photo-enhanced capabilities. Analogous materials,  $\text{NiCo}_2\text{S}_4$  and  $\text{NiCo}_2\text{Se}_4$ , are also explored to adjust the bandgap. Notably,  $\text{NiCo}_2\text{Se}_4$  displays a lower overpotential in the oxygen evolution reaction compared to  $\text{NiCo}_2\text{S}_4$  and  $\text{NiCo}_2\text{O}_4$ . Meanwhile,  $\text{NiCo}_2\text{S}_4$  exhibits a lower onset potential in the oxygen reduction reaction than  $\text{NiCo}_2\text{O}_4$  and  $\text{NiCo}_2\text{Se}_4$ . Importantly, the variances in band gap properties among these materials play a pivotal role in influencing and enhancing photoelectrochemical performances, ultimately enhancing zinc-air battery efficiency. This research contributes valuable insights to advance materials for more efficient energy conversion technologies.

**Keywords:** Oxygen evolution reaction, oxygen reduction reaction, bifunctional photoelectrocatalysts, and Zn-air batteries

# Unveiling Enhancements in Ultrathin Coating Layers on Ni-Rich NMC811 Thick Electrodes for Improved Electrochemical Performance

Surat Prempluem<sup>a</sup>, Thitiphum Sangsanit<sup>a</sup>, Kan Homlamai<sup>a</sup>, Nichakarn Anansuksawat<sup>a</sup>  
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## Abstract

Lithium-ion batteries are becoming increasingly popular due to their high energy density. However, developing cathode materials that can achieve this property while being stable and low-cost is still challenging. Ni-rich cathodes are one promising solution, but they can be unstable due to several factors, including microcracking, high surface reactivity of Ni<sup>4+</sup>, phase transformation, and thermal runaway. In this study, we demonstrate that alumina ultrathin coating improves the stability of Ni-rich thick electrodes. Atomic layer deposition (ALD) is a technique that can be used to deposit ultrathin films with sub-nanoscale thickness. The ALD coating is homogeneously distributed throughout the electrode, providing a protective layer inhibiting oxygen lattice releasing and microcracking. The results of our study show that the ALD coating can significantly improve the cycling stability of Ni-rich thick electrodes. The coated electrode retained 62% of its capacity after 498 cycles, while the uncoated electrode only retained 24%. This is a promising approach for developing high-performance and stable lithium-ion batteries.

*Keywords: Lithium-ion batteries, Ni-rich cathodes, Atomic layered deposition, Alumina*



## Study of perovskite $\text{Mn}_3\text{O}_4/\text{NiMnO}_3$ nanomaterial for supercapacitor applications

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### Abstract

In this research, pure  $\text{NiMnO}_3$  (NMO) and  $\text{Mn}_3\text{O}_4/\text{NiMnO}_3$  nanostructures have been synthesized by hydrothermal method and then were fabricated as supercapacitor. All materials were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), Transmission electron microscopy (TEM). The electrochemical performance of these nanostructures were investigated by cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS). Results showed that the NMO displayed a high specific capacitance of 262.15 F/g, while the highest enhancement by  $\text{Mn}_3\text{O}_4$  was 574.85 F/g at the scan rate of 5 mV/s and cyclic stability for 400 cycles showed results revealed that specific capacitance does not decrease, in 1 M KOH electrolyte.

*Keywords: Supercapacitor, Perovskite,  $\text{NiMnO}_3$ , nanomaterials, Energy storage*

## Microcracking of Ni-rich Layered Oxide Does Not Occur at Single Crystal Primary Particles Even Abused at 4.7 V

Kan Homlamai<sup>a</sup>, Nichakarn Anansuksawat<sup>a</sup>, Nattanon Joraleechanchai<sup>a</sup>, Poramane Chiochan, Thitiphum Sangsanit<sup>a</sup>, Worapol Tejangkura<sup>a</sup>, Thana Maihom<sup>b</sup>, Jumras Limtrakul<sup>c</sup>  
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### Abstract

The issue of particle cracking in Ni-rich layered oxide cathode materials is a source of ongoing debate in the field. There is disagreement as to whether this cracking occurs primarily at the level of individual particles or at the grain boundary. Our research, however, suggests that microcracking of NMC811 does not take place at the level of single crystalline primary particles, even when these particles are subjected to severe upper cell voltage of 4.7 V and gas evolution. This is due to the superior mechanical stability of single-crystal NMC811. Furthermore, our findings indicate that the electrochemical performance of practical full-cell level of 18650 with NMC811 cathode and graphite anode is notable. Specifically, we found that the capacity retentions at 1C rate and a 100% state of charge (SOC) were 80% and 50% after 1000 cycles for single crystal and polycrystal NMC811, respectively.

*Keywords: Li-ion batteries, Single-crystal, Ni-rich cathode, NMC811, Gas-evolution,*

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### Reference

Homlamai, K., Anansuksawat, N., Joraleechanchai, N., Chiochan, P., Sangsanit, T., Tejangkura, W., ... & Sawangphruk, M. (2022). Microcracking of Ni-rich layered oxide does not occur at single crystal primary particles even abused at 4.7 V. *Chemical Communications*, 58(81), 11382-11385.

# Nanocomposite Cathode for Sodium Ion Batteries: Single-Step Precipitation Synthesis of Prussian Blue/Reduced Graphene Oxide with Ascorbic Acid

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## Abstract

Sodium-ion batteries (NIBs) are beginning to emerge as alternatives to lithium-ion batteries (LIB) for low-cost and large-scale applications. Prussian blue (PB) is a promising cathode material for NIBs were proposed due to the similar working mechanisms with LIBs. There is also a limitation in poor electrical conductivity that decreases the effectiveness. In our work, Prussian blue (PB)/reduced graphene oxide (PB/rGO) composites are synthesized via a one-pot hydrothermal technique with different rGO contents, using ascorbic acid as a reducing agent to convert graphene oxide (GO) to rGO. PB/rGO coin cell exhibit a discharge capacity of 91 mAh g<sup>-1</sup> at 25 mA g<sup>-1</sup> with excellent rate performance and superior capacity retention remaining 84% after 1,000 cycles, shows of rGO has improved the efficiency electrochemical performance of the electrode. Including rGO conductive additives can considerably enhance the charge-discharge storage capacity and the electrode's stability. The use of battery-type cathodes presents.

*Keywords: Prussian blue, Ascorbic acid, Reduced graphene oxide, Sodium-ion batteries*

## Reducing Intrinsic Drawbacks of Ni-rich Layered Oxide with a Multifunctional Materials Dry-coating Strategy

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### Abstract

In this study, we present a novel approach for coating  $\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$  (NMC811) with a multifunctional dry coating strategy at 1 wt.% with a thickness of ca. 100 nm. For instance, the inclusion of high chemical stable  $\text{Al}_2\text{O}_3$  (at 0.33 wt.%) minimizes parasitic reactions, high electrical carbon black (also at 0.33 wt.%) helps reduce internal charge transfer resistance, and high ionic conductive  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  (at 0.33 wt.%) enhances  $\text{Li}^+$  diffusion. Employing a scalable dry coating mechanofusion process results in smoother surfaces for the spherical NMC811 particles, thereby bolstering overall stability. Remarkably, the encapsulated NMC811 cell, which boasts mixed multifunctional materials, can perform up to 1,000 cycles with 80% capacity retention. In contrast, the pristine NMC811 cell can only maintain 39%. Furthermore, the coated NMC811 provides a two-fold specific capacity at a high C-rate (2.0C) compared to the pristine counterpart. This multifunctional coating concept also offers excellent safety based on the UN38.3 standard at 18650 cylindrical cells. In light of these results, this multifunctional coating strategy may hold promise for further developing high-performance Li-ion batteries.

**Keywords:** *Electrochemical Energy storage, Li-ion batteries, Cathode, N-rich layered oxide materials, and Mechanofusion*

## Impact of cationic molecular length of ionic liquid electrolytes on cell performance of 18650 supercapacitors

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### Abstract

The charge storage mechanism of neat room temperature ionic liquids (RTILs) on electrified surfaces is uncertain, as it differs from the Gouy-Chapman theory. [1, 2] Bazant et al. proposed a model for electrochemical double layer capacitors (EDLCs) involving RTILs, addressing over screening and crowding effects [1]. A recent theoretical model suggested a charge storage mechanism in neat RTILs, indicating double layers with cationic and anionic charges at negative and positive electrodes, respectively [3]. In this study, we further explored the impact of the molecular length of RTIL cations. We synthesized RTIL electrolytes with different cationic lengths, ranging from 0.76 to 1.08 nm, encompassing ethyl to pentyl groups (C2IMI-TFSI to C5IMI-TFSI). These were all based on imidazolium structures with the same bis(trifluoromethyl sulfonyl)imide (TFSI) anion. Employing these RTIL electrolytes, we investigated their application in practical 18650 cylindrical supercapacitor cells. Notably, we employed widely-accepted, commercially available activated carbon with well-defined micro-porosity to discern the impact of cationic molecular length. Our findings indicate a linear correlation between the specific cell capacitance, equivalent series resistance (ESR), and equivalent distributed resistance (EDR) of porous carbon-based supercapacitors, all with the molecular length of the cation in room-temperature ionic liquids. [4]

*Keywords: Ionic liquid, Cationic molecular length, 18650 supercapacitors*

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# Non-flammable Electrolyte for Practical Ni-rich Li-ion Batteries with Zero Risk in Battery Explosion and Thermal Runaway

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## Abstract

This study examines the properties and applications of flame-retardant esters (FREs), specifically triethyl phosphate (TEP) and tributyl phosphate (TBP), in electrolytes. The investigation focuses on their utilization as additives (30% v/v) and main solvents (80% v/v) in conjunction with carbonate-based electrolytes (1.0 M LiPF<sub>6</sub> in EC:DEC:EMC) and a novel non-flammable electrolyte formulation (1.2 M LiPF<sub>6</sub> in 70% v/v TEP with 30% v/v fluoroethylene carbonate, FEC). The findings demonstrate that incorporating FREs as additives compromises cell performance and elevates the risk of flammability, necessitating alternative approaches for achieving nonflammability. However, employing FREs as main solvents alongside the carbonate solvents exhibits promise for the development of non-flammable electrolytes, albeit concerns such as reductive decomposition render it unsuitable for certain battery cells. Conversely, the combination of 70% v/v FREs with 30% v/v FEC in the new electrolyte formulation yields a stable solid electrolyte interface that inhibits FRE decomposition and maintains battery cycling performance. This combination presents a potential solution to produce non-flammable electrolytes, serving as a viable alternative to solid-state electrolytes. The compatibility of the 1.2 M LiPF<sub>6</sub> in TEP:FEC, 70:30 % v/v formulation with existing battery manufacturing processes further enhances its applicability. The newly developed non-flammable formulation holds promise for next-generation high-energy batteries, potentially rivalling all-solid-state electrolytes.

*Keywords: Energy storage, Li-ion batteries, Non-flammable electrolytes, Fluoroethylene carbonate, Triethyl phosphate*

## The Failure Mechanism of Large-Scale 18650 Lithium–Sulfur Batteries

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### Abstract

The emergence of lithium–sulfur batteries as an appealing alternative to conventional lithium-ion batteries is marked by their theoretical energy density of 2,500 Wh/kg, cost-effectiveness, and reduced environmental impact. However, their commercial viability is hampered by technical challenges including Li dendrite growth, insulating S cathodes, active material reduction, electrode detachment, and polysulfide shuttling. These obstacles lead to inefficiencies, compromised cycling performance, and potential failure. This research provides an in-depth exploration of upscaling LSBs to the production of 18650 cylindrical cells on a pilot plant scale. The study thoroughly investigates key challenges, optimization methods, and resulting performance and stability outcomes. The primary objective is to facilitate the practical and scalable realization of LSB technology, evaluating the feasibility of transitioning from coin cells to the 18650 format. An essential discovery pertains to a significant failure mode observed in cylindrical Li–S battery cells, characterized by considerable capacity degradation during the galvanostatic charge–discharge process due to electrode corrosion, electrolyte decomposition, and pronounced polysulfide shuttling. This endeavor serves as a substantial contribution to the advancement of energy storage solutions tailored for practical applications.

*Keywords: Lithium-sulfur battery, large-scale, cylindrical cell, 18650, failure mechanism*

## Graphite Unleashed: Natural vs. Artificial in Boosting Ni-rich Li-ion Batteries Across Coin and Cylindrical Configurations

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### Abstract

This research critically evaluated the performance of artificial graphite sourced from four eminent companies: A, B, and two variants from C (natural and artificial). A standout result emerged: C's artificial graphite demonstrated superior capacity, rapid charging, and remarkable capacity retention compared to its commercial counterparts. Notably, the specific capacity of C's artificial graphite peaked at 338.97 mAh/g, surpassing the capacities of A (321.16 mAh/g), B (314.43 mAh/g), and C's natural graphite (328.08 mAh/g). High C-rate tests (2C-5C) further accentuated C artificial graphite's exemplary capacity. After enduring 500 cycles, it retained an impressive 91.18% of its capacity, which stands in stark contrast to A's 89.44%, B's 78.78%, and C's natural graphite at 84.16%. The distinguishing performance of C's artificial graphite can be attributed to its refined characteristics, including a smaller particle size, minimal graphite imperfections, and a high 2H phase content. This reduced size permits the integration of more active material in the anode, enhancing the battery's capacity. Concurrently, fewer imperfections signify less material degradation during cycling, leading to a consistent capacity retention. In summary, C's artificial graphite emerges as a frontrunner for lithium-ion batteries, outshining commercial alternatives in efficiency and cost-effectiveness.

*Keywords: Graphite, Anode materials, Lithium-Ion Battery*



## Biochar-supported Pd Electrocatalysts for Ethanol Oxidation Reaction in Basic Medium

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### Abstract

Fuel cells such as Direct Ethanol Fuel Cell (DEFC) have attracted attention as one of the renewable sources of energy. The use of ethanol as a fuel in DEFC devices is greatly preferred due to its high availability and sustainability, low cost, easy handling, storage and transport management, and fewer hazard concerns.

Platinum (Pt) is commonly used as electrocatalysts for fuel cells due to its high electrocatalytic activity as anode materials for the oxidation of fuels (e.g., ethanol oxidation reaction (EOR)) and as cathode materials for oxygen reduction reaction (ORR). However, its use is limited by its high cost, low availability, and prevalent catalytic poisoning. Thus, numerous studies have highlighted the reduction or replacement of Pt catalyst.

Although significant improvements on the catalytic performance and cost-effectiveness of Pd-based electrocatalysts were brought about by innovations such as dispersion of nano-Pd particles on high surface area conducting support matrices (e.g., carbon black and graphene) and addition of co-metals to form bifunctional electrocatalysts, there are still interests for developing cost-effective carbon-supported Pd electrocatalysts. Biomass from agricultural wastes is now seen as a low-cost and sustainable precursor for the preparation of carbon-based nanomaterials that could be used as electrocatalyst support for DEFCs.

In this work, we have utilized agricultural biomass (e.g., rice straw and corncob) as alternative and sustainable carbon support materials for Pd-based anode electrocatalysts for ethanol oxidation reaction (EOR) in basic medium. We have investigated the physical properties of the synthesized Pd/Biochar using XRD, XPS, SEM-EDX, TEM-EDX, among others. The electrocatalytic activity and stability towards EOR were evaluated using CV and Chronoamperometry in basic medium. The electrochemical performance of the biochar-supported catalysts was compared with the commercial Pd/C.

*Keywords: biochar, Pd electrocatalyst, ethanol oxidation reaction, direct ethanol fuel cells*

# The Effects of Severe Operating Temperature on Supercapacitors

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## Abstract

In various applications, notably within the aerospace industry, supercapacitors must maintain optimal performance under low operating temperatures. The operational temperature range of supercapacitors thus becomes a crucial characteristic to consider. This study delves into the electrochemical performance and the deterioration of both electrodes and electrolytes in 18650 cell configuration supercapacitors before and after subjecting them to extreme operating temperatures by liquid nitrogen, simulating the demanding conditions encountered in aerospace applications. Our findings reveal a minor decline in the electrochemical performance of supercapacitors, primarily attributable to electrode degradation. Specifically, exposure to liquid nitrogen triggers the glass transition of the styrene butadiene rubber binder within the electrode, resulting in reduced adhesion of the active materials

*Keywords: Supercapacitors, Supercapacitors operating temperature, Electrode degradation*

## Biochar and Polypyrrole on Natural Woven Fabrics as Electrodes for Symmetrical Supercapacitors

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### Abstract

Supply of non-renewable energy resources are slowly dwindling, while also harming the environment. A promising alternative is to use natural waste material as energy sources. These waste materials can become carbon material which can be usable for typical energy storage devices such as supercapacitors, fuel cells, batteries; to name a few. Fabric materials may serve as the base of the electrode, in which the Philippines is known for its diverse range of indigenous materials. In this study, a combination of carbon materials from rice straw, with conducting polypyrrole (PPy) on indigenous fabrics as the base materials, were used for the fabrication of electrode materials for supercapacitors.

Rice straw was pyrolyzed at 700°C, and the product was treated with nitric acid, producing the locally produced activated carbon. Biochar (BC) was dispersed together with SDS, Super P® Carbon and distilled water to produce the dispersion. Both cotton (*Gossypium hirsutum*) blended fabrics of abaca (*Musa textilis*) and water hyacinth (*Eichhornia crassipes*) were separately dipped into the biochar dispersion, and subsequently brought to *in situ* chemical polymerization to coat with polypyrrole (PPy), to produce the PPy/BC/ACF and PPy/BC/WHCF composites. The resulting fully decorated electrodes were characterized using fabricated four-point probe, scanning electron microscopy, Fourier transform infrared spectroscopy, and three-electrode cyclic voltammetry (CV). The electrodes were then assembled into a symmetrical coin cell supercapacitor to perform two-electrode CV, electrochemical impedance spectroscopy, and Galvanostatic charge-discharge tests.

The micrographs for both abaca-cotton (ABF) and water hyacinth-cotton (WHCF) show RBC coating the entirety of the fabric, and that globular PPy forming on and around the biochar particles and showed good conductivity values. The 2-electrode cyclic voltammogram of the abaca fabric showed areal capacitance value of 779.13 mF/cm<sup>2</sup>, while the water hyacinth fabric gave of 643.06 mF cm<sup>-2</sup> areal capacitance. For galvanostatic charge discharge (GCD) the specific energy 13.09 Wh/kg and the specific power 1358.69 W/kg were obtained for the PPy/RBC/AC. For PPy/RBC/WHCF, it exhibited specific energy of 4.60 Wh/kg and specific power of 68.92 Wh/kg. The solution resistance for the abaca fabric was 1.52 Ω, while the charge transfer resistance was 1.71 Ω. The water hyacinth fabric solution resistance was 14.60 Ω and the charge transfer resistance was 2.79 Ω. After 10,000 cycles, the PPy/RBC/ACF composite has only retained 49% of the areal capacitance, while the PPy/RBC/WHCF composite areal capacitance exhibited retention values of around 96 – 99%. These results indicate the positive and complementary effect of the carbonaceous materials with PPy, which shows the great potential of biochar as an electrode material for supercapacitor applications.

**Keywords:** polypyrrole, fabric supercapacitor, water hyacinth, abaca, rice straw biochar

## Graphene-Based Fiber Electrode for Flexible Zn-Ion Battery

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### Abstract

Development of wearable energy storage systems has become a crucial issue due to the rapid growth of wearable electronic market such as smart textiles, artificial skin, and real-time physiological monitoring devices. One of the most successful battery systems that attains the majority of energy storage market is Li-ion battery (LIB). However, transforming LIBs into wearable energy storage devices faces big challenges in terms of flammable-electrolyte encapsulation, complicated assembly processes and limited material supply. Therefore, alternate battery systems are desired to replace current portable LIB, which are mostly unsafe and costly. Zn-ion battery (ZIB) is one of the promising energy storage systems for wearable electronic applications since they can be operated with aqueous electrolytes and assembled in ambient conditions. However, current major technical challenges that hinder industrial-scale fabrication of ZIBs are unsatisfactory electrochemical performance and unsuitable configuration for wearable applications. In this work, facile and cost-effective wet spinning technique is applied for graphene-based fiber fabrication. After chemical treatment, the graphene fibers are decorated with ion storage materials, gamma-manganese dioxide, to obtain fiber cathode. The cathode is then assembled into a cable-shaped Zn-ion battery by using the  $\gamma$ -MnO<sub>2</sub>-coated rGO fiber cathode, Zn wire anode, and xanthan gum polymeric gel electrolyte with ZnSO<sub>4</sub> and MnSO<sub>4</sub> salts. The cable-shaped ZIB presented promising maximum capacity of ~230 mAh/g with moderate cycling stability and high flexibility by maintaining the potential after consecutive pressing for 200 times under controlled testing conditions. Finally, a H<sup>+</sup>/Zn<sup>2+</sup> co-intercalation mechanism in ZIB with  $\gamma$ -MnO<sub>2</sub> materials is proposed.

**Keywords:** Fiber electrode, Zn-ion battery, Manganese dioxide, Wet spinning, Dip coating

## Electrochemical development of $\text{MnFe}_2\text{O}_4$ ferrite oxide and $\text{Mn}_3\text{O}_4/\text{MnFe}_2\text{O}_4$ nanomaterials for supercapacitor.

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### Abstract

In this research, pure  $\text{MnFe}_2\text{O}_4$  spinel ferrite oxide and  $\text{MnFe}_2\text{O}_4/\text{Mn}_3\text{O}_4$  heterostructures were explored and applied as the supercapacitor materials. These materials were fabricated by cyclic microwave method. All materials were characterized by the X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM). The electrochemical properties of materials were employed the potentiostat to study. The cyclic voltammetry showed the pure  $\text{MnFe}_2\text{O}_4$  has a capacitance of 61.83 F/g where the  $\text{Mn}_3\text{O}_4$  enhanced  $\text{MnFe}_2\text{O}_4$  was 625.74 F/g. The electrochemical impedance spectroscopy (EIS) showed that  $\text{MnFe}_2\text{O}_4$  with  $\text{Mn}_3\text{O}_4$  enhanced have a low resistance when compared to the pristine  $\text{MnFe}_2\text{O}_4$ .

*Keywords: Supercapacitor, Spinel,  $\text{MnFe}_2\text{O}_4$ , Capacitance, Heterostructures*

## Modified cellulose-based binders for aqueous-electrolyte supercapacitor

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### Abstract

We present a novel approach utilizing non-fluorinated binding material in supercapacitor electrode processing. The binders derived from acid-catalyzed conversion of carboxymethyl cellulose (CMC) or hydroxy propyl cellulose (HPMC) offer both electrode integrity and flexibility upon thermal curing at elevated temperatures. Activated carbon-based electrodes were fabricated through the integration of modified cellulose (CMC-AC or HPMC-AC) and systematically characterized for their performance in aqueous electrolyte with comparison against the polytetrafluoroethylene (PTFE-AC).

The synthesized binders demonstrated water-insolubility and chemical stability in acidic or neutral electrolyte. Fourier-transform infrared (FTIR) analysis revealed a heterogeneous furan-based materials with rich in functional groups, contributing to their superior binding performance. In 1 M H<sub>2</sub>SO<sub>4</sub> electrolyte, the maximum specific capacitance achieved using CMC-AC and HPMC-AC was measured to be 146±13 F/g and 142±9 F/g for respectively, comparable PTFE-AC capacitance of 142±9 F/g. Remarkably, all binder systems exhibited a capacitance retention of up to 85% after 1,000 cycles of charge/discharge. In summary, modified cellulose binders were presented as environmentally friendly alternatives to PTFE for electrode fabrication in aqueous-electrolyte supercapacitors. Our findings pave the way for more sustainable energy storage solutions while maintaining competitive electrochemical performance.

**Keywords:** CMC, HPMC, Binder, Supercapacitor, Aqueous electrolyte

## Electronic and electrochemical properties of $\text{Li}_2\text{XO}_3$ ( $\text{X} = \text{Mn}, \text{Cr}$ and $\text{Fe}$ ) cathodes: Spin-polarized density functional theory

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### Abstract

$\text{Li}_2\text{MnO}_3$  is one of the cathode materials for Li-ion battery applications due to high capacity and almost high voltage. In this work, the electronic and electrochemical properties of  $\text{Li}_2\text{XO}_3$  ( $\text{X} = \text{Mn}, \text{Cr}$  and  $\text{Fe}$ ) cathodes are calculated by the spin-polarized density functional theory with Hubbard type of correction (DFT+U). For the computational results, cell volumes, band gaps, density of states, stability voltages and energy barriers against  $\text{Li}^+$  transfer are demonstrated. The results indicate that the electronic and electrochemical properties are sensitive with types of the transition metals.  $\text{Li}_2\text{CrO}_3$  and  $\text{Li}_2\text{FeO}_3$  cathode are suitable to design the Lithium-rich layered transition metal oxides.

*Keywords: spin density functional theory, cathode, Li-ion diffusion, electronic properties, electrochemical properties*

## Influence of Sintering Temperatures on the Thermoelectric Properties of Ag<sub>2</sub>Se

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### Abstract

Ag<sub>2</sub>Se-based thermoelectric material shows a high thermoelectric performance at near room temperature and have considerable applications. In this work, we studied the influence of the sintering temperature for fabricating Ag<sub>2</sub>Se material on thermoelectric properties. Ag<sub>2</sub>Se pellets were prepared by wet mechanical alloying followed by cold pressing and sintering. By adjusting the sintering temperature from 403 K to 463 K thermoelectric properties changed significantly. At the sintering temperature of 403 K, the electrical resistivity, Seebeck coefficient, and thermal conductivity were  $\sim 9.5 \mu\Omega\text{m}$ ,  $\sim -138 \mu\text{VK}^{-1}$ , and  $\sim 1.06 \text{ Wm}^{-1} \text{ K}^{-1}$  at 383 K, respectively. It leads to the maximum figure-of-merit of  $\sim 0.73$  at 383 K. However, the maximum power factor of  $\sim 2374.8 \mu\text{Wm}^{-1} \text{ K}^{-2}$  at 383 K was found when the sintering temperature of 463 K was used. Therefore, the different sintering temperatures of Ag<sub>2</sub>Se have a greatly important effect on the thermoelectric properties.

*Keywords: silver selenide, thermoelectric properties, cold pressing, sintering*



## Study of the thermoelectric efficiency of Ag<sub>2</sub>Se compound via cold sintering process

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### Abstract

The study of efficient thermoelectric materials near room temperature is crucial in pathway to utilize thermal energy at low temperature. In this work, an orthorhombic silver selenide (Ag<sub>2</sub>Se) compound was synthesized to be used as the n-type thermoelectric material. Ag<sub>2</sub>Se was synthesized via wet ball milling method within 1 hour, using n-heptane to distribute Ag<sub>2</sub>Se powders. Afterward, it was cold-sintered by using dimethyl sulfoxide (DMSO) as a solvent with the concentration of 4, 6, 8 and 10 wt%. Using DMSO as the liquid medium helps rearranging the particles of Ag<sub>2</sub>Se, consequently affecting the grain size and sample density. Since the boiling point of DMSO is at 189 °C, cold sintering at 190 °C can evaporate it. Then, there are porosities between particles which vanish during increasing pressure. From thermoelectric properties measurement, it was found that the Seebeck coefficient was -153 to -115  $\mu\text{VK}^{-1}$  at 30 to 110 °C and classified as an n-type semiconductor. The electrical conductivity was increased when the concentration of DMSO was increased. The highest ZT value was around 0.9 which was Ag<sub>2</sub>Se at the concentration of 8 wt% DMSO. The lowest of thermal conductivity was 0.68 to 0.95  $\text{Wm}^{-1}\text{K}^{-1}$  at 30 to 110 °C of Ag<sub>2</sub>Se at the concentration of 6 wt% DMSO. However, the ZT was not enhanced significantly compared to Ag<sub>2</sub>Se which was added by DI water as a solvent.

*Keywords: Ag<sub>2</sub>Se, DMSO, Cold sintering process, Thermoelectric properties*

## Tailoring Structural and Electrochemical Properties by Structural Tuning of Ni/V Layered Double Hydroxide

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### Abstract

Recently, layered double hydroxides (LDHs) of transition metals have been extensively studied for energy storage applications because of their unique two-dimensional layered structure, high structural tunability, environmentally friendly nature, cost-effectiveness, and outstanding electrochemical performance. However, their unique property of intrinsic structural tunability by varying metal ion ratios still needs to be explored for the investigation of physicochemical and electrochemical properties. In this study, Ni:V LDHs were fabricated using a facile one-step hydrothermal process with different molar ratios of N:V=5:1, 3:1, 1:1, 1:3, and 1:5. XRD and FTIR analyses confirmed the successful synthesis of LDHs and confirmed the presence of free hydroxyl groups when V<sup>3+</sup> was the dominant dopant. SEM images showed increasing crystallinity when Ni<sup>2+</sup> was dominant, whereas increasing the ratio of V<sup>3+</sup> caused a decrease in crystallinity owing to the presence of more hydroxyl groups. Ni:V=1:1 showed the highest areal capacitance (Ca) of 4451 mF cm<sup>-2</sup> at the current density of 4 mA cm<sup>-2</sup>, but poor capacitance retention of 67% after 1000 cycles at a constant current density of 15 mA cm<sup>-2</sup>. Ni-dominant LDHs, Ni:V=3:1 and 5:1 showed Ca of 732.5 and 3317 mF cm<sup>-2</sup> with capacitance retentions of 102% and 91% respectively. In the case of V-dominant, Ni:V=1:3 showed Ca of 2034 mF cm<sup>-2</sup> and capacitance retention of 43%, whereas Ni:V=5:1 showed Ca of 950.0 mF cm<sup>-2</sup> and capacitance retention of 56%. Thus, the Ni:V= 3:1, and 5:1 LDHs exhibited high areal capacitance with improved cycling stability owing to their high crystallinity, whereas the Ni:V=1:3 and 1:5 LDHs showed low areal capacitance and poor cycling stability due to low crystallinity but exhibited high conductivity.

*Keywords: Layered Double Hydroxides, Hydrothermal Process, Areal Capacitance, Cycling Stability, Energy Storage*

# Catalytic Hydrothermal Carbonization of Biomass to Porous Carbon for Electrochemical Energy Storage

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## Abstract

One of the most promising technologies for synthesizing solid carbons at moderate temperatures and regulated saturated water pressure is hydrothermal carbonization (HTC). Although high-pressure water has particular advantages as a reaction medium during HTC, paths of the hydrothermal reaction can be further tailored by catalysts for the desired carbon properties. This contribution proposes a simple but effective method for producing hydrochar from biomass such as water hyacinth. Pretreatment of the biomass was conducted by HTC under the catalysts, including acetic acid, zinc chloride, and phosphoric acid. The solid carbons were characterized by SEM, XRD, IR, N<sub>2</sub>-sorption and elemental analysis, demonstrating a well-developed graphitic carbon and porosity. Then, the biochar from an appropriate HTC condition was further activated at a high temperature. The resulting carbon has a large surface area (1353 m<sup>2</sup> g<sup>-1</sup>) and up to 80% of micropores, making it appropriate for energy storage devices. When the activated carbon was used as an electrode material in a symmetric supercapacitor, it showed a high specific capacitance of 93 F g<sup>-1</sup> at a current rate of 0.5 A g<sup>-1</sup>, which is 20% greater than a commercially activated carbon. [1] This sustainable procedure for producing highly porous carbon is practical for implementation in the energy storage device, emphasizing the SDGs in terms of converting waste into high-value products and affordable energy for everyone.

**Keywords:** *Hydrothermal carbonization, Activated carbon, Acetic acid, Supercapacitor*

[1] Butcha, S., et al. "Sustainable production of multifunctional hierarchical carbon from weed water hyacinth: Assessment for lithium-ion battery and supercapacitor." *Journal of Energy Storage* 72 (2023): 108578.

# Unlocking the Mysteries of Metal Dissolution: Understanding Consequences and Pioneering Solutions

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## Abstract

Lithium-ion batteries, renowned for their unparalleled energy density and longevity, are pivotal in driving modern technology, from electric vehicles to ubiquitous devices like laptops and smartphones. Central to their functionality is the orchestrated movement of lithium ions between electrodes, generating electricity. This dance sees the anode, primarily graphite, in concert with a cathode harnessing transition metal oxides, including cobalt, manganese, or nickel. During the charging phase, lithium ions traverse from anode to cathode, reversing the journey upon discharge. Yet, a lurking challenge overshadows this intricate ballet: the instability of transition metal oxides, culminating in their potential dissolution into the electrolyte over charge-discharge cycles. To probe this phenomenon, we employed cylindrical lithium-ion batteries (18650) with a distinctive jelly roll design, paired with a meticulously chosen 1.2M LiPF<sub>6</sub> EC: EMC: DEC: FEC (1:1:1:1.3%v) electrolyte composition. Deliberately overcharging the batteries to varying voltage levels, we harvested electrode samples for rigorous analysis. Utilizing Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES), we uncovered a direct relationship between increased overcharge voltage and escalated metal dissolution at the anode, with the zenith observed at 4.9V. This metal dissolution surge is ascribed to voltage-triggered electrolyte decomposition, yielding byproducts adept at dissolving transition metal oxides. Our research posits the strategic adoption of modified electrolytes as a vanguard against metal dissolution, heralding the next era of more resilient and secure lithium-ion batteries.

*Keywords: Lithium-ion batteries, Metal dissolution, Graphite, Inductively Couple Plasma Optical Emission Spectroscopy (ICP-OES) and Organic electrolyte.*

# Unlocking the Secrets of Supercapacitor Performance: Acetamide as the Molecular Indicator of Electrolyte Decomposition

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## Abstract

Acetonitrile (ACN)-based electrolytes in supercapacitors exhibit intricate decomposition pathways including hydrolysis, polymerization, Hofmann elimination, and fluorination reactions. Such molecular phenomena significantly impede electrolyte and electrode performance, leading to pore obstruction, gas evolution, capacity reduction, and heightened resistance. Central to these processes is the electrolyte's water content, which instigates the transformation of ACN into acetamide, thereby diminishing the electrode surface area. Our study employed a cylindrical supercapacitor 18650, integrated within a 'jelly roll' system. Utilizing 1 M tetraethylammonium tetrafluoroborate (TEABF<sub>4</sub>) in an ACN electrolyte and activated carbon (AC) electrode, we varied voltage from 2.7 V to 4.1 V over a 12-hour period. Analytical techniques, notably nuclear magnetic resonance (NMR) and gas chromatography-mass spectrometry (GC-MS), were deployed to discern molecular changes. Initial findings revealed the fresh electrolyte's water content at approximately 20 ppm, which escalated under heightened voltage conditions. Peak acetamide concentrations were observed at 3.5 V, tapering post this threshold. Intriguingly, by 3.7 V, N-ethyl acetamide concentrations surged with voltage increments. This research underscores not only the electrolyte's role but also the electrode's contribution in water origination, necessitating deeper exploration for optimized supercapacitor performance.

*Keywords: Supercapacitor, Activated carbon, tetraethylammonium tetrafluoroborate, electrolyte decomposition*

## Effect of $\text{Cu}^{2+}$ and $\text{Ca}^{2+}$ on Dielectric Properties Variation in $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ Ceramic

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### Abstract

In this study on dielectric properties change with Cu increase of  $\text{CaTiO}_3$  material, the formula is  $\text{Ca}_{1+x}\text{Cu}_{3-x}\text{Ti}_4\text{O}_{12}$  ceramic with increase  $\text{Ca}^{2+}$  and decrease  $\text{Cu}^{2+}$  ( $x = 0, 1, 1.5, 2$  and  $3$ ) were prepared using a solid-state reaction method. X-ray diffraction technique was used to confirm the phases of  $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$  and in terms ( $x \geq 1$ ) the second phase of  $\text{CaTiO}_3$  phases was detected in ceramics. The in the grain of all ceramics can be observed using scanning electron microscopy and can confirm the occurrence of the second phase of  $\text{CaTiO}_3$  using an Energy Dispersive X-ray spectroscopy. The results revealed that ceramics sintered at  $1060^\circ\text{C}$  for 8 h exhibited increased dielectric permittivity when the conditions with the highest Cu content  $x=0$  ( $\sim 26,000$  at 1 kHz) but in this condition have the highest dielectric loss tangent (0.145) and On the other hand, the dielectric value decreased with decreasing Cu content. We can found the  $\text{CaTiO}_3$  phase when the addition of Ca resulted is decreased dielectric loss tangent was very low (0.006 – 0.010 at 1 kHz).

*Keywords: second phases, Dielectric properties*

# AC-Driven electroluminescent devices fabricated using Nb<sup>5+</sup>-doped TiO<sub>2</sub> nanostructured ceramics

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## Abstract

This research delineates the successful fabrication of AC-Driven Electroluminescent (EL) Devices utilizing 1% and 5% Nb<sup>5+</sup>-Doped TiO<sub>2</sub> Nanostructured Ceramics as a pivotal dielectric layer, paving the path for innovative advancements in electronic device applications. The ceramics were meticulously prepared through the conventional mixed oxide method, marking a significant improvement over their undoped counterparts in the composition of electroluminescent devices. An in-depth characterization of the synthesized powders was undertaken, employing X-ray diffraction and transmission electron microscopy to ascertain their structural and morphological attributes. A comparative analysis revealed that both 1% and 5% doped TiO<sub>2</sub> ceramics demonstrated superior performance when integrated as a dielectric layer in AC-Driven EL devices, as opposed to the utilization of undoped TiO<sub>2</sub>. Moreover, the photoluminescence properties of the fabricated devices were systematically evaluated, further corroborating the enhanced functionality rendered by the doped ceramics. This groundbreaking study underscores the potential of Nb<sup>5+</sup>-Doped TiO<sub>2</sub> Nanostructured Ceramics in revolutionizing the fabrication of AC-Driven Electroluminescent devices, offering promising prospects for the development of new-generation electronic devices with augmented capabilities and applications.

*Keywords: Rutile-TiO<sub>2</sub>, AC-Driven electroluminescent devices, Nanostructure*

# Nanostructured $\text{Na}_{1/2}\text{Y}_{1/2}\text{Cu}_3\text{Ti}_4\text{O}_{12}$ ceramics with giant dielectric properties

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## Abstract

The dielectric material  $\text{Na}_{1/2}\text{Y}_{1/2}\text{Cu}_3\text{Ti}_4\text{O}_{12}$  (NYCTO) was synthesized using the solid-state reaction method. A comparative study was conducted between a conventional ball mill and a high-energy ball mill, both operated at 1000 rpm for 30 minutes. Nanostructured  $\text{Na}_{1/2}\text{Y}_{1/2}\text{Cu}_3\text{Ti}_4\text{O}_{12}$  Ceramics were revealed using transmission electron microscope. X-ray diffraction analyses revealed the presence of a single NYCTO phase. Scanning electron microscopy examination confirmed the homogeneity of the material's grains, and Energy-Dispersive X-ray Spectroscopy was used to analyze the elemental composition. High-energy ball milling allowed for a reduction in the sintering temperature. Consequently, sintering was carried out at 1020°C for 6 hours under high-energy ball mill conditions, resulting in the highest dielectric value (7300 at 1kHz) and a dielectric loss of approximately 0.1 at 1kHz.

**Keywords:** Dielectric properties, high energy ball milling



## Dielectric Properties of CuO/TiO<sub>2</sub> Nanocomposite

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### Abstract

Composite (1-x)CuO/xTiO<sub>2</sub> ceramics (x = 0%, 10%, 20%, 30%, 40%, and 50%) were prepared using a solid-state reaction method. X-ray diffraction was employed to confirm the presence of second phases of CuO and TiO<sub>2</sub>. The grains of all ceramics were observed using scanning electron microscopy, and the composite between CuO and TiO<sub>2</sub> was confirmed using Energy Dispersive X-ray Spectroscopy. The results revealed that under the condition of pure CuO, the highest dielectric permittivity was observed (24000 at 1kHz at room temperature). However, in the case of the composite with TiO<sub>2</sub>, a decrease in dielectric permittivity and dielectric loss was observed. The humidity sensing properties of this material were studied in the relative humidity range of 30-90%. Our results showed an improvement in the capacitive absorption of water molecules.

*Keywords: Humidity sensing, Dielectric permittivity, Composite ceramics*

# Enhanced Dielectric Properties of Nanostructured Ta<sup>5+</sup>-Doped TiO<sub>2</sub> Ceramics through SnF<sub>4</sub> Addition and High-Energy Ball Milling

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## Abstract

In this study, we synthesized  $TiO_{0.9}Ta_{0.1}O_2$  powders with different doping concentrations utilizing the high-energy ball milling method.  $SnF_4$  nanoparticles were integrated into the  $Ta^{5+}$ -doped  $TiO_2$  ceramics, facilitating enhanced density at reduced sintering temperatures. The ceramic particles were characterized using transmission electron microscopy. The sintered ceramic samples were analyzed systematically through a variety of techniques, including X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and Raman spectroscopy. We investigated the notable dielectric properties as functions of frequency, temperature, and DC bias. The influence of  $SnF_4$  on the evolution of the microstructure, electrical properties, and dielectric behavior was discussed.

**Keywords:** Nanoparticles; TiO<sub>2</sub>; High energy ball milling; Microstructure; Giant dielectric constant

# Leveraging Nanotechnology for Green Mitigation Change and Effects on Environment and Agriculture

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## Abstract

The need for long-term, creative responses to climate change has grown as the globe struggles to cope with its worsening effects. This talk covers nanotechnology's potential as a climate-friendly instrument for softening the blow of global warming on the natural world and the agricultural sector. The possibilities of carbon capture and storage, renewable energy, energy efficiency, water treatment, and climate-resilient agriculture using nanomaterials and nanotechnology will be explored. Carbon nanotubes, metal-organic frameworks, graphene, and catalysis nanomaterials are examples of nanomaterials with special qualities that can be used to better sequester carbon dioxide, generate and store renewable energy, purify water, and cultivate crops with pinpoint accuracy. The possible environmental and health risk linked with nanomaterials must be taken into account, even while nanotechnology offers promise green solutions.

*Keywords: Nanotechnology, Green mitigation change, Nanomaterial, Environment, Agriculture*

## ประวัติและผลงาน (CV)



### 1. ประวัติส่วนตัว

ชื่อ-สกุล ศาสตราจารย์ ดร. พวงรัตน์ แก้วล้อม (ขจิตวิชยานุกุล)  
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Research gate (Impact point = 26.74); Google Scholar (H-index = 22)  
ความเชี่ยวชาญ สารเคมีตกค้างในอาหารและสิ่งแวดล้อม การแปรรูปของสารเคมีในสิ่งแวดล้อม  
การฟื้นฟูดินเสื่อมสภาพ การจัดการน้ำ เทคโนโลยีสีเขียว ระบบนิเวศเกษตรอินทรีย์

### 2. ประวัติการศึกษา

- ปริญญาเอก PhD in Civil and Environmental Engineering, The University of Texas at Arlington  
ประเทศสหรัฐอเมริกา (พ.ศ.2544)
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- ใบอนุญาตประกอบวิชาชีพวิศวกรรมควบคุมสาขาสิ่งแวดล้อม ระดับภาคีวิศวกร

## Removal of Iodinated Disinfection by-Products by Modified Metal-Organic Frameworks

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### Abstract

The application of modified metal-organic frameworks (MOFs) for eliminating emerging iodinated disinfection by-products (I-DBPs) to increase water safety—affected by the lack of clean water resources and seawater intrusion—was investigated. The I-DBPs removal efficiencies of MOFs—MIL-53(Al), MIL-88B(Fe), UIO-66(Zr), ZIF-8(Zn), and HKUST-1(Cu)—modified by the thiol functionalized on a coated silica layer, and pyrolysis at 700 °C and 900 °C, were studied. The removal mechanisms in single- and mixed-solute solutions caused by their physicochemical properties (i.e., thermal stability, crystallinity, porosity and surface area, elemental analysis, active surface functional groups, hydrophobicity, and morphology imaging) and their relationship with adsorption rate and capacities were described. The direct post-grafting of dithioglycol to the metal complex node (e.g., ZIF-8 and HKUST-1) promotes synergetic adsorptive interactions consisting of Lewis acid–base interaction via the metal complex, ion-dipole interactions involving protonated hydroxyl and thiol groups, and hydrophobic interactions at the organic linkers. Interestingly, the dehalogenation of triiodomethane to diiodomethane due to nucleophilic substitution ( $S_N2$ ) reactions can be accelerated by the thiol-functionalized silica layer on ZIF-8. Meanwhile, MIL-88B(Fe)-derived carbon at 900 °C (CMIL88-900) greatly increased in surface area, porosity, and hydrophobicity, resulting in excellent adsorption rates and capacities of five I-THMs (4–44 times, calculated by linear isotherm) compared to powdered activated carbon (PAC). The primary adsorptive mechanisms onto CMIL88-900 consist of hydrophobic partitioning and an ion–dipole interaction at the acidic surface functional groups (ASGs), which is supported by the diffusibility of the small molecular structure of I-THMs. Chlorinated haloforms showed a higher adsorption capacity on CMIL88-900 than brominated and iodinated haloforms. Due to its hydrophobicity and low molecular weight, dichloriodomethane had a higher adsorption capacity on CMIL88-900 than iodoacetic acid and iodoacetamide.

**Keywords:** Thiol-functionalized MOFs, MOF-derived carbon, iodinated disinfection by-products, adsorption, dehalogenation

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- 2009 to 2013 : Assistant Professor , Department of Environmental Engineering, Faculty of Engineering, Chulalongkorn University.
- 2013 to present : Associate Professor , Department of Environmental Engineering, Faculty of Engineering, Chulalongkorn University.

#### **Fields of Specialization:**

- Adsorption Process for Water and Wastewater Engineering
  - Removal of emerging micro-pollutants by using adsorption process.
  - Adsorption mechanisms analysis
  - Surface modification for enhance of emerging micro-pollutants adsorption capacities.
  - Removal of disinfection by products (DBPs) using modified mesoporous silicates.
- Wastewater Collection and Treatment
  - Physical-chemical process for industrial wastewater treatment.
- Water Supply Engineering
  - Disinfection by products (DBPs)
  - Water reuse
- Environmental Impact Assessment
- Industrial Waste Management and Utilization

# Towards Environmental Sustainability: Synthesis and Scale-up of MOFs from Recycled Materials for Environmental Applications

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## Abstract

The rapid rise of non-biodegradable plastics and waste metals poses an imminent global threat that requires urgent attention. Sustainable and green technologies are crucial for recycling these materials into value-added products. Among the many value-added products, metal-organic frameworks (MOF) are of particular interest to researchers and industrial sectors due to their unique properties such as permanent porosity, high surface area, structural flexibility, and tailored functionality. The versatility of MOFs finds applications across diverse fields such as carbon capture, gas storage, gas separation, sensing, and heterogeneous catalysis, resulting in a growing demand. One of the factors delaying the entry of MOFs into the market is their synthesis, which often requires expensive materials. Utilizing waste-derived resources as a dependable source for both organic and inorganic elements is an alternative to solving production costs. In addition, implementing circular economy principles, which involve cost reduction, waste reduction, and minimizing environmental impact, would greatly enhance the feasibility of mass MOF production. This approach would extend the benefits of MOFs to practical real-world applications. Herein, we address an innovative large-scale synthesis of MOF derived from waste employing flow chemistry as well as an example use of MOFs for environmental applications.

*Keywords: Metal-organic frameworks, Circular economy, Large-scale production, Sustainable synthesis, Environmental applications*

### Short Bio:

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### Education

The University of Texas at Dallas, Texas, USA — Postdoctoral associate, 2011  
Integrated water gas shift membrane reactors utilizing novel, non-precious metal mixed matrix membrane  
The University of Texas at Dallas, Texas, USA — Ph.D./Chemistry, 2010  
Functionalized TiO<sub>2</sub> nanotubes and their applications  
Texas A&M University-Commerce, Texas, USA — M.S./ Chemistry, 2006  
Development of Ni/Al<sub>2</sub>O<sub>3</sub> catalysts via the RF plasma technology for benzene hydrogenation  
Chulalongkorn University, Bangkok, Thailand — B.S./Chemistry, 2002  
Synthesis of redox-active bis(calix[4]quinoxines) and their electrochemical properties

### Field of Specialization

Fabrication of heterogeneous catalysts, reactor design, and catalyst treatment with radio-frequency plasma.  
Synthesis and characterization of organic/inorganic nanomaterials (metal oxide nanotubes, MOFs and quantum dots).  
Research experience in preparation and characterization of mixed matrix membrane for gas/ liquid separation

### Research Interest

Synthesis of porous nanomaterials for energy production and environmental cleanup.  
Fabrication of membranes for gas or liquid separation.  
Synthesis of heterogeneous catalysts and design of catalytic membrane reactor

### Selected Publications

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## Innovative Graphene Oxide-Nile Red Fluorescent Dye for Identification and Quantitation of Microplastics

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### Abstract

This research aims to present an innovative application of graphene oxide (GO) as a nanomaterial mixed with Nile Red (NR) for detecting microplastics. The problem of microplastics is important to significant environmental pollution due to their potential to harm the environment and attract chemical pollutants. Previous techniques were used for surveying and monitoring microplastic pollution in the environment generally involved large-sized instruments, expensiveness, and time-consuming for analysis. Additionally, the fluorescent staining process involving NR-GO required a digital image-based method for the analysis of microplastics. The optimized mixing ratio of NR-GO dye was a 1:1 of NR to GO by volume, resulting in the improvement of the fluorescent intensity. The NR-GO dye was successfully applied to stain five types of microplastics. Microplastics exhibiting a fluorescent signal with NR-GO staining could be classified into three groups: yellow for polyethylene (PE) and polypropylene (PP), red for polyethylene terephthalate (PET), and orange for polyvinyl chloride (PVC) and polystyrene (PS). The variation in fluorescent colors depended on the microplastic functional groups. The color intensity, as indicated by the Red Green Blue (RGB) intensity data, was obtained from fluorescent image captures of each microplastic type using the developed software program in a portable fluorescence device. Under optimal conditions, the calibration curve for PE was established within the range from 0.1 to 1.2 mg with a linear regression coefficient of 0.99. Moreover, a portable fluorescence device was applied to determine microplastics in the water sample. Hence, this innovative microplastic device demonstrated the effectiveness for identification and quantitation of microplastics.

*Keywords: Graphene Oxide, Nile red, Microplastics, Image Processing, Color Intensity*

## Enhancing the TDS Removal in Sedimentation Process by Graphene Magnetic Property

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Tippabust Eksangsri<sup>b</sup>

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<sup>b</sup> Department of Chemical Engineering, Faculty of Engineering, Thammasat University, Thailand,

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### Abstract

Seawater intrusion occurs every year, causes high salinity or high Total Dissolved Solid (TDS) to fresh water. This also affects the water quality especially as the problem happening in Chao Pa Ya River, Thailand. This problem can be harmful to human as the use of tap water for drinking water. Reverse Osmosis (RO) process is the possible method to solve this problem. However, cost of investment is quite high including operation and maintenance cost. Moreover, application of the RO process can be used only for short period of time during the intrusion of seawater. In which, this might not be economically feasible. Nowadays, graphene applications are using for water purification as adsorbent or part of membrane. Magnetic property of graphene from Magnetic Graphene Oxide (MGO) is aimed assisting the strong bonding of adsorption process and enhancing rapidly settlement of solid for TDS removal. Synthesis of graphite to graphene by Modified Hammer's method and adding magnetic property with  $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$  and  $\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$  solution were applied. Results from adsorption showed that removal percentage of TDS in synthesized NaCl water at pH 7 was up to 70% with the equilibrium time at 10 mins. The experiments also revealed that the optimum dosage of MGO adsorbent was 20 mg in synthesized water of 20 mL with the NaCl concentration of 1,800 mg/L. Therefore, the settling time between using and not using the magnet were 3 mins and more than 20 mins, respectively. This rate could be applied in the sedimentation process and help reduced the sedimentation tank. In summary, the application of magnet property of MGO could be the promising technology for treating TDS water and solving the salt problem in drinking water.

*Keywords: Adsorption, Magnetic Graphene Oxide, Sedimentation process, Total Dissolved Solid*

# Synthesis of Graphene from Agricultural Waste for Electrodes in Capacitive Deionization Applications

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## Abstract

Capacitive deionization (CDI) has received increasing interest as a solution for freshwater shortage because of its low energy requirement and lower cost compared to other methods. In CDI technique, two electrodes are oppositely biased so that  $\text{Na}^+$  and  $\text{Cl}^-$  ions are moved to each electrode by Coulomb force and then absorb at surface of electrodes. Carbon materials are considered as one of the promising candidates for electrodes in CDI because of their large surface area, high conductivity and high chemical stability, but CDI performance may be limited by their hydrophobicity. In this study, reduced graphene oxide (rGO) is focused on because its hydrophilic surface, in addition to large surface area and low electrical resistance is expected to give increased salt absorption capacity compared to other carbon electrodes. Conventionally, rGO is synthesized by reducing graphene oxide (GO) obtained from Hummers' method, using graphite as starting material. In this study we used biochar derived from agricultural waste such as sugarcane bagasse and hemp hurds through dehydration reaction with concentrated  $\text{H}_2\text{SO}_4$ , as starting material for Hummers' method because this can lower the cost and can offer a possibility for up cycling agricultural waste.

In biochar synthesis, the weight-to-volume ratio between biomass and concentrated  $\text{H}_2\text{SO}_4$  were varied. The obtained biochar was then oxidized into graphene oxide by modified Hummer's method and then reduced by ascorbic acid solution. The physicochemical properties of the product from each step were investigated by Raman spectroscopy and Fourier transform infrared spectroscopy. The specific surface area of the samples was investigated by  $\text{N}_2$  adsorption-desorption isotherms. CDI of NaCl solution using rGO as electrodes was successfully conducted. Salt adsorption capacity of each rGO electrodes were investigated by conductivity measurement during CDI with varied initial concentration of NaCl solution. The results will be discussed in detail in the presentation.

*Keywords: Graphene, Reduced graphene oxide, Biomass, Hummers' method, Dehydration*

## A Study on Superhydrophilic and Anti-Dust Coatings Using Mixed Colloidal Silica Nanoparticles

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Nutkritta yimpun<sup>b</sup>, Narin Chomcharoen<sup>a</sup>, Pisist Kumnorkaew<sup>a</sup> and Tanyakorn Muangnapoh<sup>a,\*</sup>

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### Abstract

In the past decade, nanotechnology has captured the attention of researchers and industries due to its potential to add more value to original materials. Thin film coating via nanomaterials can provide new properties and enhance the performance of pristine surfaces for specific applications. The development of solution-based coatings from inorganic/organic solutions and colloidal systems could benefit industries due to much lower costs in material production and a less complicated coating protocol. In this study, we fabricated a coating using colloidal silica nanoparticles with sizes ranging from 12 to 45 nm. We tailored the surface properties by varying volumetric ratio of two dispersed sizes of silica nanoparticles, aiming to achieve a superhydrophilic and anti-dust coating while preserving the coating's transparency. The results of the experiment revealed that a silica sol solution containing two dispersed sizes of silica nanoparticles led to a water droplet contact angle of less than 10°, coupled with excellent light transmittance similar to the bare glass surface. In addition, the dust adhesion test on the coated surface demonstrated effective dust protection, with a visible light transmission (%VLT) greater than 80%.

*Keywords: Superhydrophilic, Anti-dust, Silica nanoparticle, Contact angle*

## Development of plastic composites with virucidal efficacy for pandemic preparedness

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<sup>a</sup>*School of Energy, Materials & Chemical Engineering, Korea University and Technology and Education, 1600 Chungjeol-ro, Byeongcheon-myeon, Dongnam-gu, Cheonan-si, Chungcheongnam-do (31253), Republic of Korea*

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### Abstract

In light of the COVID-19 outbreak, there has been an increasing interest in investigating the antiviral properties of commonly used plastics. The primary route of virus transmission is through indirect contact between infected and uninfected individuals *via* surface. Therefore, it is imperative to infuse plastic products in public spaces, where numerous individuals come into contact indiscriminately, with virucidal properties. While antimicrobial copper products are available on the market, they suffer from the drawback of copper oxidation over time, leading to the formation of copper (II) oxide, which lacks effectiveness against viruses. To overcome this limitation, the present study aims to develop composites by incorporating visible light-responsive photocatalysts into silicone and polypropylene (PP), thereby creating commercial plastic products with sustained virucidal efficacy. These plastic products could potentially find utility in public places or medial institutions, aiding preparedness for future pandemics.

*Keywords: copper oxide, photocatalysis, visible light, virucidal, pandemic preparedness*

## Mechanical and Dielectric Properties of Fly Ash Geopolymer/Sugarcane Bagasse Ash Composites

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### Abstract

Waste from lignite power plants and sugar industries, fly ash (FA) and sugarcane bagasse ash (SCBA) are usually disposed of as landfills. In this research, these wastes were effectively utilized as a construction material, namely geopolymer. The investigation was the effect of the addition of SCBA (0-40 wt.%) to the FA geopolymers. The compressive strength of the FA geopolymers was reduced with the addition of SCBA. This reduction was primarily attributed to the presence of the highly stable and non-reactive quartz (SiO<sub>2</sub>) phase in SCBA. The SCBA was not dissolved in the alkaline-activated solution and did not play a role in the geopolymerization process. In the geopolymer matrix, the unreacted SCBA particles remained present without contributing to strength. Nevertheless, when the SCBA quantity was approximately 10 wt.% or lower, the effects on the properties of FA geopolymers were minimal. Furthermore, the dielectric properties of the FA geopolymer/SCBA composites were also investigated in this research. The pristine geopolymer displayed a relatively large dielectric constant ( $\epsilon' = 3.6 \times 10^3$ ). The addition of SCBA decreased the  $\epsilon'$  slightly due to the high carbon content in SCBA. However, the primary influence on the  $\epsilon'$  variation was governed by the geopolymerization process, facilitating the formation of the aluminosilicate gel structure.

*Keywords: fly ash, sugarcane bagasse ash, geopolymer, dielectric properties, mechanical properties*

## Photocatalytic Degradation Study of Methylene Blue by Dumbbell-like $\text{TiO}_2$ Capped Gold Nanorods under UV and NIR irradiation

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Navadecho Chankhunthod<sup>a,b\*</sup>

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### Abstract

Enhancing the photocatalytic efficiency of titanium dioxide ( $\text{TiO}_2$ ) can be achieved through a unique approach involving a two-interface system consisting of metal- $\text{TiO}_2$  interfaces. This approach has received significant attention in research, with gold nanorods (AuNRs) being an interesting point due to their ability to be tuned in term of size and shape via controlled synthesis methods. Their unique plasmonic properties called surface plasmon resonances (SPR) further contribute to their appeal. Semiconductor coated AuNRs were illustrated high electron transfer efficiency. This is because, at interfaces, AuNRs is connected to electron acceptor enhancing electron charge transfer resulting in higher photocatalytic activity. In this research, the synthesized tunable AuNRs and the  $\text{TiO}_2$  coated AuNRs were fabricated and characterized using UV-vis spectroscopy, TEM, and TEM-EDX. The effect of silver ion on AuNRs synthesis and the influence of CTAB concentration on the  $\text{TiO}_2$  coating process were discussed. Photocatalytic activity of methylene blue (MB) degradation was analyzed under UV and NIR irradiation. It was found that photocatalytic activities were most prevalent under UV light irradiation, illustrating a 51.3 % degradation of dye. In contrast, NIR-irradiation displayed slightly lower degradation rate, at 50.0%. Interestingly, simultaneous UV and NIR irradiation led to only a 16.9% degradation rate. This suggests that our developed nanostructures hold potential as effective photocatalysts within  $\text{TiO}_2/\text{Au}$  systems, advancing wastewater treatment applications in the future.

*Keywords: Gold nanostructures, Photocatalyst, Titania, Dye degradation*

# Microporous Membrane in Preparation from Layered Double Hydroxide on Graphene Oxide Nanosheet for the Efficient Water Decontamination

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Saifon Kullyakool<sup>a</sup>, Sandhya Babel<sup>b</sup>

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## Abstract

Graphene oxide nanosheet was incorporated with CaFeAl-based layered double hydroxide (LDH) via in situ chemical co-precipitation to earn a uniform hybrid nanomaterial composite. A series of LDHs prepared with different ratios of divalent and trivalent cations were in attempts where the results of these preparations were evaluated systematically. The surface properties are the crucial keys focused for material development. In this work, the resulting hybrid nanostructure products of LDH and GO were promisingly made and transformable into the microporous membranes with assisting bi-polymer formulation in enhancing stability. Its surface properties of the dried form were characterized before and after its combining with the mixed hydrophobic polymers. Further but with primarily studies when equipped with an in-house developed filtration module, this LDH/GO nanohybrid membrane performed a surprising performance in decontaminating chloride ion in a short time as well as other ions from the tested ground water samples.

*Keywords: Nanoclay, Filtration, Adsorption, Hybrid, Removal*



# De-risking a Metal-Organic Framework for Practical Carbon Capture

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## Abstract

Metal-organic frameworks (MOFs) are transcending from fundamental to applied research, but their use in a large-scale process has not yet been realized. For many industrial uses, MOFs face a challenge of economical performance in a durable, scalable material implementable in an appropriate engineered form. This presentation will deal with two short stories spanning our efforts to design new porous solids while keeping an eye on real-world applications.

MOFs can be used like a sponge to trap selected gases and release them under some external stimulus (e.g., pressure drop, temperature increase). Such an approach has been challenging for post-combustion carbon capture owing to the presence of water and acid gases in the stream. CO<sub>2</sub>. We have developed a solid [1] that has moved up the technology ladder, with different academic and industrial partners, to actually be capturing CO<sub>2</sub> industrially at 25 tonnes per day scale. This talk will discuss some of the basic science and also the hurdles to translate from milligrams to industrial demonstration including the key aspect of being able to physisorb CO<sub>2</sub> in the presence of water.[2]

The second part will deal with a new approach to make MOFs. MOFs typically rely on a reticular (net-based) approach where metal and organic linkers define a topology and pore sizes. We have developed a new route to highly stable MOFs [3] where the guest molecules can play a much greater role in structure determination - rather than simply filling the void, determining its structure. This approach relies on robust H-bonded intermediates. Results on the use of this approach for xylene isomer separation will be presented. [4]

[1] Shimizu, G. K. H., Rajendran, A., Woo, T. K. and coworkers, *Science* 2021, 374, 1464.

[2] Shimizu, G. K. H., Rajendran, A., Woo, T. K. *Adv. Mater.* 2023, in press.

[3] Shimizu, G. K. H. and coworkers, *J. Am. Chem. Soc.* Accepted.

[4] Shimizu, G. K. H. and coworkers, 2022, PCT application.

**Short Bio: Prof. George Shimizu**

**Academic Appointments:**

Full Professor, University of Calgary, Calgary, Alberta, Canada 2007-present  
Associate Professor, University of Calgary, Calgary, Alberta, Canada 2002- 2007  
Assistant Professor, University of Calgary, Calgary, Alberta, Canada 1998- 2002

**Selected Awards / Honours**

**2021 Alberta Science and Technology Foundation (ASTech) Award for Outstanding Achievement in Energy and Environmental Innovation**  
**2019 Canadian Society for Chemistry Rio Tinto Alcan Award for Inorganic Chemistry**  
**2019 Parex Innovation Fellowship** (1 of 6 at the University in inaugural cohort)  
**2012 International Zeolite Association-Elected to inaugural MOF Committee (member to 2018)**  
**2010 University of Calgary Faculty of Science Research Excellence Award**  
**2008 Canadian Society for Chemistry Strem Award for Pure or Applied Inorganic Chemistry**  
**2008 NSERC Discovery Grant Accelerator Award**

**Bibliometric Data (based only on independent UCalgary career as Feb 2023)**

>100 papers, all in ISI journals. H-Index= 52, Citations ~13000, ~110 citations/paper. Papers as PI or co-PI include *Science* (3), *Nature Materials*, *Nature Chemistry*, *J. American Chemical Society* (13), *Angewandte Chemie* (4), *CHEM*(2), *Chemical Communications* (15), *Advanced materials* (1), *Chemistry of Materials* (6).

**High impact research contributions in the last five years:**

1. The highest impact work relates to a licensed patent and the associated paper in *Science* on a new sorbent for carbon capture. This metal-organic framework (MOF) has been capturing 1 tpd CO<sub>2</sub> from a Lafarge cement plant in Richmond, B.C. since early 2021 and 30 tpd from a Chevron plant in California since fall 2022. Our work involved the discovery, characterization, derisking and scaleup for industrial partners.
2. A PCT patent filing and second disclosure concerns a new family of highly stable MOFs with the unique ability to be templated around guest molecules to imprint their structure on the pore. Licensing negotiations are in progress.
3. A PCT patent concerns sustainable MOF superprotonic membranes and *CHEM* paper (over 10<sup>-2</sup> S cm<sup>-1</sup> conduction).
4. A PCT patent concerns merging CO<sub>2</sub> capture and conversion with Assoc *ACS Energy Lett* paper.

**Recent major grants received (PI in all cases)**

Carbon Capture Inc. Research Contract, \$240K, 2022-2024, for MOFs for direct air capture.  
Alberta Innovates Strategic Project, \$560K, 2017-2021, joint with A. Rajendran at UAlberta to research new sorbents for carbon capture.  
NSERC CREATE, \$1.05M, 2015-2019, 10 PIs for a carbon capture training program.  
NSERC CRD, \$160K, 2020-2023, with David Bromley Engineering to develop materials as coating for water purification membranes.  
NSERC RTIs (2): 2020 for Dynamic Sorption Analyzer (\$150K) for competitive sorption of mixed gases and in 2021(\$149K) for a six-station gas sorption analyzer.

**Invited, Keynote and Plenary Lectures:**

- More than 120 invited talks at conferences including keynote or plenary talks at: Gordon Conference on CCUS (2023, Switzerland); Telluride Conference on Porous Solids (2023, Colorado); ( MOF2022 (Dresden); Fundamentals of Adsorption 14 (2022, Colorado); Materials for Humanity (2021, Singapore); Internat'l Conf. Intercalation Chemistry (2019 Sao Paulo, Brazil); Can Soc Chem Eng (2017 Edmonton), BC Inorganic Discussion Weekend (2015 Squamish); Internat'l Symp on Solid State Ionics (2015, Colorado), Ontario/Quebec Cryst. Eng Emerg. Mater. Workshop Ont/Que (2015- Guelph); NANO-VII (2014-Niagara Falls); MOF2014 (2014-Kobe); Internat. Symp. Zeolites Micropor. Cryst. (2012- Hiroshima); Eur. Conf. Chem. Mol. Sci. (2012 Prague).
- More than 95 invited talks in Canada, Japan, China, USA, France, India, Saudi Arabia.

# Harnessing Electroactivity in Metal-Organic Frameworks: Fundamentals to Applications

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## Abstract

Electroactive Metal-Organic Frameworks (MOFs) offer a powerful platform to explore electron transfer phenomena within 3-dimensional coordination space. At the applied level, these materials have enormous potential as the basis for electrocatalysts, porous conductors, batteries and solar energy harvesting systems, amongst numerous other potential applications.<sup>1</sup>

This presentation will overview our team's research in electroactive MOFs that integrate molecular components for electron transfer and their stimuli responsive properties.<sup>2-4</sup> Key to our investigations have been solid-state AC/DC electrochemical methods and near-IR/Vis, EPR, FT-infrared and Raman spectroelectrochemical (SEC) techniques developed in our laboratory,<sup>1</sup> providing powerful in situ probes for the optical and electron transfer characteristics of MOFs. Our experimental work is supported by theoretical and computational modelling, providing insights into the mechanisms and kinetics of charge transfer phenomena.

Harnessing their electroactive properties has enabled us to develop new porous semiconductors, electro- and photo-catalysts, all-optical and photothermal conversion devices, and novel methods for gas separations based on 3D printed MOFs.<sup>5-6</sup> Our latest work with Australian renewables start-up company Southern Green Gas will be described,<sup>7</sup> including our advances in green synthesis to technoeconomic analysis and 3D printing for prototyping. The context for this interdisciplinary and intersector project within the broader Net Zero Initiative will also be described.

## Selected References:

1. D. M. D'Alessandro, *Chem. Commun.* 2016, 52, 8957-8971.
2. R. Murase, T. Hudson, T. Aldershof, K. Nguyen, J. Gluschke, E. Kenny, X. Zhou, T. Wang, M. van Koeven, B. Powell, A. Micolich, B. Abrahams, D. M. D'Alessandro, *J. Am. Chem. Soc.* 2022, 144, 13242-13253.
3. D. A. Sherman, R. Murase, S. G. Duyker, Q. Gu, W. Lewis, T. Lu, Y. Liu, D. M. D'Alessandro, *Nature Commun.* 2020, 11, DOI: 10.1038/s41467-020-15510-7.
4. C. Hua, P. W. Doherty, B. Ding, B. Chan, M. Yu, D. M. D'Alessandro, *J. Am. Chem. Soc.* 2018, 140, 6622-6630.
5. T. Wang, R. Sabatini, B. Chan, J. Hou, V. Huynh, N. Proschogo, Z. Xie, L. Gao, J. Zhang, B. Hawke, R. Clarke, C.J. Kepert, V. Chen, G. Lakhwani, D. M. D'Alessandro, *ACS Materials Lett.* 2021, 3, 1599-1604.
6. E. R. Kearns, R. Gillespie, D. M. D'Alessandro, *J. Mater. Chem. A* 2021, 9, 27252-27270.
7. D. M. D'Alessandro, *The Conversation*, 2021, <https://theconversation.com/engineers-have-built-machines-to-scrub-co-from-the-air-but-will-it-halt-climate-change-152975>

**Short Bio: Deanna M. D'Alessandro**

Net Zero Initiative Website: <https://net-zero.sydney.edu.au/>

Research Group Website: <https://www.deannadalessandrogroup.com/>

Current appointment: Professor & Director, Net Zero Initiative, The University of Sydney. Joint appointment between Faculty of Engineering (School of Chemical & Biomolecular Engineering) and Faculty of Science (School of Chemistry).

Qualifications: B.Sc. (Hons I, U. Medal), James Cook University (JCU), 2001; PhD, 2006.

**Relevant employment history:**

American Australian Association DOW Chemical Company Fellow & Royal Commission for the Exhibition of 1851 Research Fellow (University of California, Berkeley) 2007-2009; USyd Postdoctoral Fellow 2010; L'Oréal Australia for Women in Science Fellow 2010; Australian Research Council (ARC) QEII Fellow 2011-2016\*; Associate Professor 2017-2020; Deputy Head of School (Chemistry) & Inaugural Chair Equity, Diversity & Inclusion Committee 2017-2018; SOAR Fellow 2017-2018; ARC Future Fellow 2018-2022\*, Professor 2021-present; Director, Net Zero Initiative 2023-2026. {\*3 years of career interruptions for maternity leave and part-time employment}

**Major Professional Recognitions:**

2023 Royal Society of Chemistry Australasian Lectureship  
2017 Le Fèvre Medal, Australian Academy of Science  
2017 Fellow, Royal Australian Chemical Institute  
2017 Alan Sargeson Lectureship, Royal Australian Chemical Institute (Inorganic Division)  
2015 ChemComm Emerging Investigator Lectureship, Royal Society of Chemistry  
2014 Rennie Memorial Medal, Royal Australian Chemical Institute  
2012 Distinguished Lectureship Award, The Chemical Society of Japan  
2011 NSW Young Tall Poppy Science Award, Australian Institute of Political Science  
2007 International Union of Pure and Applied Chemistry (IUPAC) Prize for Young Chemists  
2007 Cornforth Medal, Royal Australian Chemical Institute

Selected Major Competitive Funding (past 10 years): Musk Foundation XPRIZE in Carbon Removals (Student Team Prize), Direct Air Capture (US\$250k, 2022); ARC Future Fellowship, Harnessing Electroactivity in Metal-Organic Frameworks (\$860k, 2018-22, sole-CI); ARC DP, Putting Metal-Organic Frameworks to Work at Interfaces (\$463k, 2018-21, co-CI); Sydney Research Accelerator Research (SOAR) Fellowship, USyd (\$100k, 2017-18, sole-CI); ARC DP, A Radical Approach to Multifunctional Coordination Solids (\$483k, 2015-17, lead-CI); ARC DP, Advanced Functional Properties in Metal-Organic Framework Materials" (\$420k, 2012-2014, co-CI); CSIRO Science and Industry Endowment Fund, Solving the Energy Waste Roadblock (\$6M, 2011-16, co-CI); ARC QEII Fellowship, Conducting Nanoporous Materials: toward Molecular Devices (\$788k, 2011-16, sole-CI).

Selected Major Invited Presentations (past 10 years): Plenary Lecture, NZ National Chemistry Congress, Auckland, NZ (2022); Keynote Lecture, MOFweb The International Conference on Metal-Organic Frameworks, Online (2020); Plenary Lecture, 7th Asian Conference on Coordination Chemistry, Kuala Lumpur, Malaysia (2019); Keynote Lecture, International Conference on Coordination Chemistry, Sendai, Japan (2018); Keynote Lecture, International Symposium on Macrocyclic and Supramolecular Chemistry, Cambridge UK (2017); ChemComm Emerging Investigator Lecture, The International Chemical Congress of Pacific Basin Societies, Hawaii, USA (2015); Orica black tie dinner speaker, International Year of Chemistry Launch, Great Hall, Parliament House, Canberra (2011).

## Co-Based Metal-Organic Frameworks for Photocatalytic Hydrogen Production

Sareeya Bureekaew<sup>a,\*</sup>, Ladawan Pakdeejorhor<sup>a</sup>, and Taya Saothayanun<sup>a</sup>

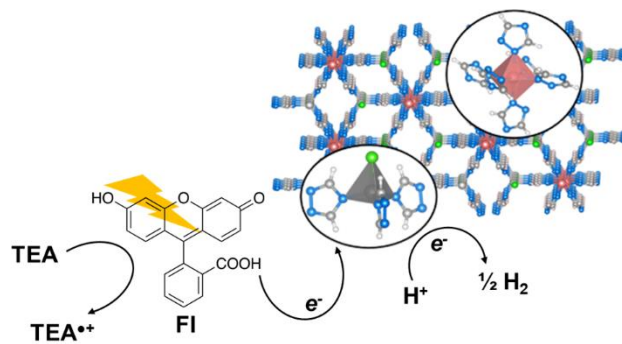
<sup>a</sup>*School of Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology (VISTEC), Rayong, 21210 THAILAND*

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### Abstract

Metal-organic frameworks (MOFs) are porous crystalline materials that hold great promise for various applications, including photocatalysis. In this study, the photocatalytic performance of highly photostable Co-based MOFs was demonstrated in the presence of fluorescein (FI) and triethylamine (TEA) as a photosensitizer and a sacrificial agent, respectively. The Co-MOFs exhibit two distinct Co centers—one responsible for catalytically active functions and the other for conductivity—resulting in effective hydrogen (H<sub>2</sub>) generation through photocatalytic reactions. Factors such as morphology, substituent groups, and mixed metals on the catalytic performance will be examined and discussed.



**Figure.** Proposed mechanisms for photocatalytic H<sub>2</sub> production occurred on Co-MOF.

**Keywords:** Metal-organic framework, Photocatalyst, Hydrogen production

### Short Bio: Sareeya Bureekaew

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 Office telephone/Mobile phone +66 (0) 3301 4256  
 Educations Ph.D., Department of Biological Chemistry and Synthetic Chemistry, Graduate School of Engineering, Kyoto University, Japan

### Positions and Professional Activities

- 2015~: Lecturer, Institute of Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Rayong, Thailand
- 2013 –2015 Lee Kuan Yew (LKY) Postdoctoral Fellowship, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore
- 2009 – 2013 Postdoctoral Researcher, Ruhr-University Bochum, Germany
- 2009 – 2009 Postdoctoral Researcher, ERATO Kitagawa Integrated Pores Project. Japan Science and Technology Agency (JST), The Institute for Integrated Cell-Material Sciences(i-CeMS), Kyoto University, Japan

### Selected Publications

- (1) Suppaso, C.; Pongkan, N.; Intachai, S.; Inchongkol, Y.; Bureekaew, S.; Khaorapong, N. Tin sulfides and cadmium sulfide mixture in montmorillonite with enhanced visible-light photocatalytic activity. *Applied Clay Science* **2023**, *241*, 106999.
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- (4) Lerdwiriyanupap, T.; Cedeno, R.; Nalaoh, P.; Bureekaew, S.; Promarak, V.; Flood, A. E. Enantiopurification of Mandelic Acid by Crystallization-Induced Diastereomer Transformation: An Experimental and Computational Study. *Crystal Growth & Design* **2023**, *23* (3), 2001.
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- (7) Siwaipram, S.; Bopp, P. A.; Ponchai, P.; Soetens, J.-C.; Hasegawa, J.-y.; Schmid, R.; Bureekaew, S. MD studies of methanol confined in the metal-organic framework MOF MIL-88B-Cl. *Journal of Molecular Liquids* **2022**, *359*, 119252.
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- (9) Nulek, T.; Klaysri, R.; Cedeno, R.; Nalaoh, P.; Bureekaew, S.; Promarak, V.; Flood, A. E. Separation of Etiracetam Enantiomers Using Enantiospecific Cocrystallization with 2-Chloromandelic Acid. *ACS Omega* **2022**, *7* (23), 19465.
- (10) Kongkatigumjorn, N.; Srikamut, P.; Seidi, F.; Bureekaew, S.; Crespy, D. Tuning the Hydrolytic Behavior of Hydroxyquinoline Derivatives for Anticorrosion Applications. *Chemistry of Materials* **2022**, *34* (6), 2842.
- (11) Sattayapanich, K.; Chaiwat, W.; Boonmark, S.; Bureekaew, S.; Sutthasupa, S. Alginate-based hydrogels embedded with ZnO nanoparticles as highly responsive colorimetric oxygen indicators. *New Journal of Chemistry* **2022**, *46* (40), 19322.
- (12) Pukdeejorhor, L.; Adpakpang, K.; Wannapaiboon, S.; Bureekaew, S. Co-based metal-organic framework for photocatalytic hydrogen generation. *Chemical Communications* **2022**, *58* (59), 8194.
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# Advances in Process Design for Electrocatalytic CO<sub>2</sub> Reduction and Biomass Oxidation: From Catalysts to Functional Devices

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## Abstract

In the pursuit of global decarbonization, the chemical sector emerges as a critical focal point for transformation. Shifting away from conventional petroleum-based resources to renewable sources is imperative, and pivotal advancements lie in the utilization of CO<sub>2</sub> and biomass as renewable carbon feedstocks. Harnessing their potential for sustainable carbon sourcing can significantly curtail greenhouse gas emissions, contributing to a net-zero carbon future.

Electrochemical conversion of CO<sub>2</sub> and biomass offers an innovative pathway that outperforms traditional thermocatalysis on several fronts. By operating at lower temperatures, exhibiting faster start-up and shutdown times, and directly interfacing with renewable electricity sources, electrochemical processes stand as a promising route for clean carbon transformation. A distinctive advantage of electrochemistry is the ability to decouple reduction and oxidation processes, facilitating the concurrent production and efficient separation of multiple value-added products. Despite these promising attributes, electrochemical processes are in the early stages of development, necessitating profound insights not only into the underlying chemistry of reactions but also the intricacies of charge transfer processes at both macro and micro scales. This talk aims to elucidate our approach to the design of practical electrocatalytic systems tailored for CO<sub>2</sub> reduction and biomass oxidation. The intricate interplay of catalyst development, electrode design, and reaction engineering will be explored. Our focus extends beyond catalyst development, encompassing the strategic process design required to translate theoretical potential into functional electrochemical devices.

*Keywords: Metal-organic framework, Photocatalyst, Hydrogen production*

2023 Curriculum Vitae

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### EDUCATION

**Stanford University, Stanford, California, USA** 2011 – 2017  
Ph.D. in Chemical Engineering

**Northwestern University, Evanston, Illinois, USA** 2007 – 2011  
B.S. in Chemical Engineering, *Magna Cum Laude*

### Awards and Honors

Thesis Award (Excellence level) in Engineering from the National Research Council of Thailand 2019  
Full scholarship from the Ministry of Science and Technology of Thailand from B.S. – Ph.D. 2006 – 2017  
Stanford Graduate Fellowship Award 2011 – 2014  
RISE fellowship, granted by the German Academic Exchange Service (DAAD) 2010

### RESEARCH INTERESTS

- Electrocatalytic and photoelectrochemical systems for biorefinery, sustainable chemistry, renewable energy storage, and environmental applications
- Surface science and thin-film processing technologies

### RESEARCH EXPERIENCE

**Nanocatalysis and Molecular Simulation (NCAS) Research Group,**  
**National Nanotechnology Center (NANOTEC),**  
**National Science and Technology Development Agency (NSTDA), Pathumthani, Thailand** Oct 2017 – Present  
**Researcher**

Supervisor: Dr. Kajornsak Faungnawakij

- Led research projects in electrochemical processes for energy and environmental applications
- Designed and conducted research projects for industry solutions

**Corporate Technology Development, Lam Research Corporation, California, USA** Apr 2017 – Sep 2017  
**Process Engineer Intern**

Supervisor: Dr. Nerissa Draeger

- Conducted research projects focusing on advanced technology inflections for the semiconductor industry
- Developed deposition processes for self-assembled monolayers (SAMs) for area-selective atomic layer deposition (AS-ALD) applications

**Department of Chemical Engineering, Stanford University, California, USA** 2012 – 2017  
**Ph.D. Candidate**

Supervisor: Professor Thomas F. Jaramillo

- Fabricated a tandem photoanode capable of bias-free solar water splitting using Si processing techniques
- Investigated substrate effects on catalyst activity via *in situ* electrochemical characterizations and spectroscopy
- Constructed a LabVIEW-controlled automation for spray pyrolysis system

**Stanford Nanofabrication Facility, Stanford University, California, USA** 2015 – 2016  
**Volunteer Researcher**

- Optimized an ALD recipe for SnO<sub>2</sub> using TDMASn and water in the Savannah S200 (Cambridge Nanotech)
- Developed an ALD of WO<sub>3</sub> using (tBuN)<sub>2</sub>(Me<sub>2</sub>N)<sub>2</sub>W and O<sub>2</sub> plasma in the Fiji system (Cambridge Nanotech)



# Enhanced Ionic Conduction by Vibrational Strong Coupling of Water

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## Abstract

Here, we discuss the effect of vibrational strong coupling on the ionic conductivity of aqueous electrolytes. Even under the dark condition, the energy resonance of cavity vacuum field to the molecular vibration level leads to the vibrational strong coupling state. Interestingly, we observed significant enhancements in ionic conductivity, especially for one-order of magnitude enhancement of proton. We discuss the origin of the ionic conductivity behavior regarding to the modification of the hydration dynamics.

**Keywords:** *Vibrational strong coupling, Water, Cavity, Ionic conductivity*

The energy states of molecular vibration and the vacuum electromagnetic field can be hybridized to form a vibrational strong coupling state (VSC) (Figure 1). It has been demonstrated that VSC can be used to modify the chemical dynamics of molecules. Here, we propose that ion dynamics can be altered through modifications of the dynamic hydration structure under VSC. Infrared spectroscopy of aqueous electrolyte solutions in the cavity confirmed the occurrence of vibrational ultra-strong coupling behavior of water molecules,<sup>1</sup> even in the presence of electrolytes. Interestingly, we observed significant enhancements in ionic conductivity, especially for one-order of magnitude enhancement of proton (Figure 2).<sup>2</sup> These enhancements are both feasible and cannot be explained within the current theoretical framework for liquid electrolytes. Our analysis suggests that the vibrational strong coupling leads to the modification of local dielectric friction experienced by hydrated ions.<sup>3</sup>

By harnessing the unique properties of strong coupling and its influence on hydration dynamics, we can pave the way for the development of novel electrolytes and advancements in the field of ionic conduction.

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- (3) **T. Fukushima**, S. Yoshimitsu, K. Murakoshi, *submitted*. ChemRxiv preprint DOI: 10.26434/chemrxiv-2023-b649f

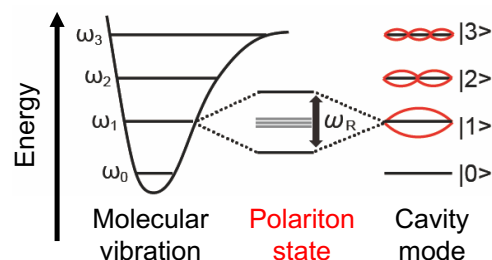


Figure 1. Energy scheme of the vibrational strong coupling between molecules and cavity.

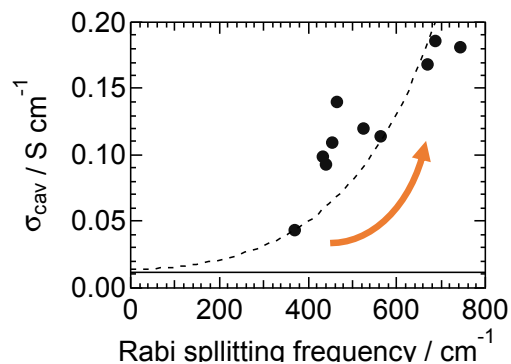


Figure 2. Effect of Rabi splitting frequency of H<sup>+</sup> conductivity in 0.01 M HClO<sub>4</sub> electrolyte in cavity.

**Short Bio: Tomohiro Fukushima, Ph.D.**

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**Professional Appointments**

Lecturer	Hokkaido University, Japan
Host: Prof. Kei Murakoshi	June 2022 – Present
Assistant Professor	Hokkaido University, Japan
Host: Prof. Kei Murakoshi	December 2017 – June 2022
Postdoctoral Associate	JST-ERATO
Host: Prof. Kenichiro Itami	Nagoya University, Japan
	June 2016 – November 2017
Postdoctoral Fellow	Japan Society for the Promotion of Science (JSPS)
Host: Prof. Yogesh Surendranath	Massachusetts Institute of Technology, United of States
	June 2014 – May 2016

**Education**

Ph.D. Engineering	Kyoto University, Japan
Thesis Title: Studies on Assemblage-Directed Functions of Porous Coordination Polymers March 2014	
Graduated Student	Kyoto University, Japan
Research Fellow (DC1)	JSPS
Supervisor: Prof. Susumu Kitagawa	April 2009 – March 2014
B. Sc. Engineering	Kyoto University, Japan
	April 2005 – March 2009

**Academic Standing**

Young Investigator Award: Japan Society for Molecular Science	2022
Oral Presentation Award: The Spectroscopical Society of Japan	2021
2014 Reaxys PhD Prize Finalist	2014
JSPS Fellowship for Research Abroad (FY 2014)	2014-2016
CSJ Student Presentation Award: 93rd Annual Meeting of the Chemical Society Japan	2013
Soft Matter Poster Award: International Association of Colloid and Interfacial Science	2012
Competitive Travel Grants: PBAST-6	2011
Research Aboard Fellowship: Kyoto University 21st Global COE Program	2011
JSPS Fellowship for Young Scientist DC1 (FY 2011)	2011-2014
JASSO Scholarship Fellowship for Excellence	2011
Poster Award: 4 <sup>th</sup> Annual Meeting of Japan Society for Molecular Science	2010
Poster Award: 60 <sup>th</sup> Anniversary Conference on Coordination Chemistry in Osaka	2010

# Utilizing the Heterogeneous Catalysts for Conversion of Oil-based Feedstocks and Platform Chemicals to Biofuel and Biochemicals in Biorefinery Applications

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## Abstract

Recently, the platform chemicals derived from lignocellulosic biomass and oil-based feedstock have been recognized as the important bioresources for an alternative production biofuel and biochemicals. Especially, on the basis of Thailand as an agricultural-based country, the successful utilization of agricultural feedstocks to replace petroleum and petrochemical products would strongly support the Bio-Circular-Green Economic Model or BCG of the country. In this present, the conversion of platform chemicals, furfural (FAL) and 5-hydroxymethylfurfural (5-HMF), and oil-based feedstock in batch and continuous operation modes were examined using the developed Cu, Ni, and Fe-based catalysts. Primarily, the bimetallic CuRe with different Cu: Re molar ratios were prepared by sequential wetness impregnation method and their catalytic activities for furfural hydrogenolysis into 2-methylfuran were examined in comparison to the monometallic Cu and Re benchmarks. Alternatively, catalytic transformation of furfural to furfuryl alcohol and 2-methylfuran without H<sub>2</sub> supply toward transfer hydrogenation process using 2-propanol as a H<sub>2</sub> source was systematically investigated over the low-cost bimetallic NiCu, CoCu, and CuFe catalysts in comparison with the monometallic Cu, Ni, Fe, and Co catalysts. Additionally, the as-synthesized  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> supported NiFe catalysts with different Ni to Fe molar ratios were developed and applied for the continuous hydrogenolysis of 5-hydroxymethylfurfural to 2,5-dimethylfuran. As for conversion of oil-based feedstock, the novel bifunctional Ni-Re supported on bimodal SAPO-11 catalyst was designed for an economically combined process of direct triglycerides hydro-deoxygenation and isomerization into low-cold flow diesel. Lastly, the catalyst characterizations by nitrogen (N<sub>2</sub>) sorption, H<sub>2</sub> temperature-programmed reduction (H<sub>2</sub>-TPR), NH<sub>3</sub> temperature-programmed desorption (NH<sub>3</sub>-TPD), Fourier transform infrared spectroscopy (Pyridine-DRIFTS), X-ray diffractometry (XRD), X-ray photoelectron spectroscopy (XPS), X-ray absorption near edge structure (XANES), Time-resolved X-ray absorption spectroscopy (XAS), and transmission electron microscopy-energy dispersive electron microscopy (TEM-EDS) were demonstrated to comprehend on the correlation between the catalytic activity and catalyst properties.

## Short Bio:

Atthapon Srifa earned his PhD in 2015 from Chulalongkorn University under the guidance of Prof. Suttichai Assabumrungrat and Dr. Kajornsak Faungnawakij and spent postdoc time with Prof. Koichi Eguchi at Kyoto University in 2015-2016. His areas of expertise and interests are mainly focused on development of heterogenous catalysts for the reactions involving with high pressure hydrogen such as hydrogenation, hydrogenolysis, hydrodeoxygenation, and isomerization in biorefinery applications. Currently, he is working as an assistant professor at Department of Chemical Engineering, Faculty of Engineering, Mahidol University, Thailand



# Simple Catalysts with Remarkable Chemistry for the Cycloaddition of CO<sub>2</sub> to epoxides

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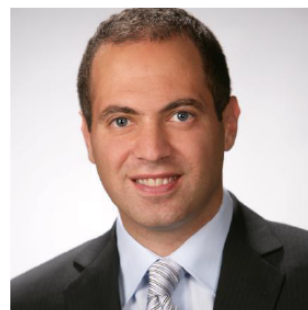
## Abstract

The cycloaddition of CO<sub>2</sub> to epoxides is a widely studied reaction because it represents a convenient way to combine CO<sub>2</sub> conversion with the synthesis of industrially attractive commodity chemicals and intermediates.[1-2] Furthermore, it can be carried out under very mild and even ambient conditions when the suitable catalytic system is employed.[3] Previously, the choice of catalysts able to efficiently promote the title reaction under ambient conditions was limited to high molecular weight metal-organic complexes requiring multistep syntheses and elaborate organic frameworks to tune the metal center.[1] Nevertheless, our work has demonstrated that simple coordination complexes of early transition metals such as Nb,[4] Y,[5] Zr[6] are efficient Lewis acids for the cycloaddition of CO<sub>2</sub> to terminal epoxides even when using flue gas CO<sub>2</sub> as the feedstock. More recently, we have been able to extend this kind of chemistry to the preparation of recyclable heterogeneous Lewis acids[7] and fully heterogeneous catalysts[8] with the ability to carry out the target cycloaddition reaction under very mild conditions. On the other hand, recent investigation by our group has involved the application of naturally available and benign organocatalysts such as ascorbic acid and its derivatives[9-11] or sodium citrate[12] acting as hydrogen bond donors for the conversion of biobased epoxides to cyclic carbonates. While these kinds of homogeneous organocatalytic components are difficult to recover from the reaction mixture, our very recent advances show that biphasic reaction conditions can be applied in the presence of suitable biobased organocatalysts to afford efficient cyclic carbonate synthesis along with catalyst recovery in a separate aqueous phase.[13] These aspects will be discussed with a focus on the mechanistic features and on the rationalization of the observed catalytic activity.

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- [13] T. Theerathanagorn, A. Vidal-López, A. Comas-Vives, A. Poater, V. D'Elia, *Green Chemistry* 2023, 25, 4336-4349.

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**Research Targets**

Catalysis and Catalytic Materials, CO<sub>2</sub> Conversion,  
Environmental Chemistry, Organic and  
Organometallic Chemistry, Nanotechnology, Oil  
and Gas, Circular Economy, Waste Conversion,  
Energy, Renewability and Sustainability

**Main Skills and Keywords**

Project management, Team Leading, Results  
Analysis and Elaboration, Organic and  
Organometallic Chemistry, Analytical and  
Organizational Skills, Proposals and Manuscripts  
Writing, Teaching Skills, Scientific Reviewer

**Achievements**

~70 Publications/Patents;  $h^{index}$ : 33; Citations>3000  
(Scopus/Google Scholar/Web of Science);

**Pages with Metrics**

<https://www.scopus.com/authid/detail.uri?authorId=57216485896> (Scopus Profile)  
<https://scholar.google.com/citations?user=M5ipiisA-AAJ&hl=de> (Google Scholar Profile)  
<https://www.webofscience.com/wos/author/record/460750>;  
<https://www.researchgate.net/profile/Valerio-D-Elia>

**Education**

**March 2005 – December 2008** Doctoral studies at the University of Regensburg, Germany (Group of Prof. Dr. O. Reiser)  
Title obtained PhD, Organic Chemistry. Result: Magna cum Laude (Exam on 8<sup>th</sup> February 2009)

**October 1995 – December 2001** Chemistry studies at the University of Perugia, Italy  
Title obtained MS degree, Chemistry. Result: 110/110 et laude (13<sup>th</sup> December 2001)

**Latest Employments with Research activities**

**July 2015 – Current** Associate Professor/Team leader at the Vidyasirimedhi Institute of Science and Technology, Rayong, Thailand  
*„Design and Application of materials and molecular catalysts for C-H and CO<sub>2</sub> activation“*

**December 2010 – July 2015** Research scientist at KCC (Kaust Catalysis Center) in the group of Prof. Dr. J.-M. Basset  
*„Synthesis of homogenous and heterogeneous catalysts for C-H and CO<sub>2</sub> activation“*

**January 2009 – November 2010** Research Scientist under the supervision of Prof. Dr. Hendrik Zipse at the LMU Munich  
*„Synthesis of immobilized organocatalysts for the esterification of tertiary alcohols“*

**March 2005 – December 2008** Research Assistant under the supervision of Prof. Dr. O. Reiser at the University of Regensburg  
*„Synthesis of short  $\alpha/\beta$ -peptides as bifunctional organocatalysts“*

**March 2002 - February 2005** Researcher at the „Dompé Farmaceutici S.p.A.“ in L'Aquila, Italy ([www.dompe.it](http://www.dompe.it))  
*„Synthesis of allosteric IL-8 receptor inhibitors“*

**Teaching activities**

(2015-) Course organizer of Chemical Thermodynamics (MSE-501) and Heterogeneous Catalysis (MSE-545) at the Vidyasirimedhi Institute. Supervision of Master and PhD Thesis.

(2010-2015) Acting Supervisor of several PhD students through their research activities and thesis at Kaust.

(2007-2009) Teaching assistant for the „Gattermann lab-course“ at the LMU Munich and University of Regensburg

## Triazole-containing catalysts for alcohol oxidation and CO<sub>2</sub> conversion

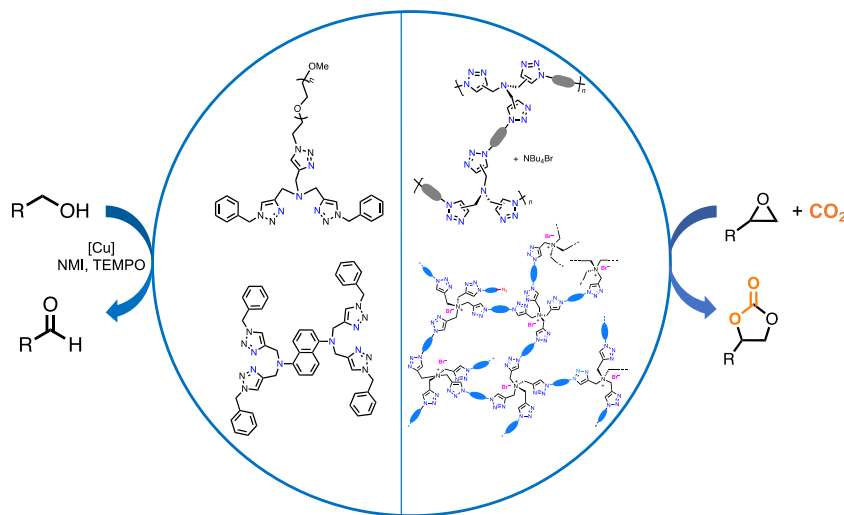
Preeyanuch Sangtrirutnugul<sup>a,\*</sup>, Vasut Nakarajouyphon<sup>a</sup>, Attawit Jehdaramarn<sup>a</sup>, Siraprapha Somsri<sup>a</sup>, Pobporn Promchan<sup>a</sup>

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### Abstract

Copper-catalyzed azide–alkyne cycloaddition (CuAAC) offers a relatively simple and effective way to combine building blocks, *i.e.*, terminal alkynes and organic azides, and give regioselective 1,4-disubstituted-1,2,3-triazole products under mild conditions. Using this method, triazole-based copper complexes and organic polymers containing various functional groups such as pyridine, amine, and quaternary ammonium groups were conveniently prepared. Through judicious design and coordination versatility of triazoles, improved catalytic activities of copper catalysts towards aerobic alcohol oxidation to aldehydes were achieved. In addition, triazole-based organic polymers were demonstrated as efficient and reusable catalysts, with and without co-catalysts, for CO<sub>2</sub>/epoxide cycloaddition to yield cyclic carbonates under mild conditions.



**Keywords:** triazole, alcohol oxidation, carbon dioxide, cyclic carbonates, catalysis

## Enhanced Syngas Production via CO<sub>2</sub> Reforming of Methane over Ni/SBA-15 Nano-Catalyst Derived from Palm Oil Fuel Ash

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### Abstract

Greenhouse gas emissions resulting from economic activities and industrial sectors primarily stem from Methane (CH<sub>4</sub>) and Carbon Dioxide (CO<sub>2</sub>). A significant approach to mitigating environmental issues caused by GHGs involves the utilization of CH<sub>4</sub> and CO<sub>2</sub> to generate syngas. Syngas, consisting of a mixture of H<sub>2</sub> and CO, serves as a valuable feedstock for the production of various chemical products and fuels. CO<sub>2</sub> reforming (CRM) has emerged as an economically viable method for syngas production and is widely employed in industries. Consequently, this research focuses on synthesizing Ni/SBA-15 and Ni/Zr-SBA-15 catalysts using Palm Oil Fuel Ash (POFA) as the silica source to form the SBA-15 support, Nickel as the active metal, and Zirconia as the promoter. The impregnation method successfully synthesized Ni/SBA-15 and Ni/Zr-SBA-15 catalysts. Characterization of the catalysts involved XPS, FESEM, and XRD analytical techniques, while the catalytic activity for CRM reaction was assessed based on CH<sub>4</sub> and CO<sub>2</sub> conversions in a tubular furnace reactor. Ni/Zr-SBA-15 exhibited improved characteristics compared to Ni/SBA-15, including enhanced stability, composition, porosity, and catalyst structure attributed to the presence of Zr. The results demonstrate that Ni/Zr-SBA-15 outperformed Ni/SBA-15 with conversion rates of 90.5% and 91.5% for CH<sub>4</sub> and CO<sub>2</sub>, respectively. Furthermore, the H<sub>2</sub>/CO ratio produced by Ni/Zr-SBA-15 was higher and closer to 1 than that of Ni/SBA-15. The results unequivocally demonstrate the significant impact of Zr support on the Ni/SBA-15 catalyst during CRM. The excellent performance of Ni/Zr-SBA-15 can be attributed to two primary factors. Firstly, the presence of an effective O<sub>2</sub>-rich surface aids in extending the interfacial boundary between the metal and support, thereby mitigating carbon deposition. Secondly, the well-dispersed small-sized Ni and Zr particles play a crucial role in preventing metal sintering, ensuring sustained catalytic activity.

*Keywords: Syngas, CO<sub>2</sub> Reforming, Greenhouse gases, POFA, Catalyst*



# In-Situ Growth of Amine-Functionalized G-C<sub>3</sub>N<sub>4</sub> Nanotubes With Carbon Vacancies Induced by Ni Single Atoms for Efficient Visible-Light Photocatalytic CO<sub>2</sub> Reduction

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## Abstract

Carbon dioxide (CO<sub>2</sub>) conversion into fuels and valuable chemicals driven by solar energy is a promising method for solving global warming and shortage of fossil-derived chemicals simultaneously. Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) has been considered as one of the most promising photocatalysts for photocatalytic CO<sub>2</sub> reduction. However, its overall performance is still relatively low due to severe recombination of electron-hole pairs. Introduction of carbon (C) vacancy is an effective point-defect engineering strategy to mitigate its electron-hole recombination, while amine groups (-NH<sub>2</sub>) in g-C<sub>3</sub>N<sub>4</sub> structure could act as an active site for photocatalytic CO<sub>2</sub> reduction. Herein, we report a novel strategy for synthesizing amine-functionalized g-C<sub>3</sub>N<sub>4</sub> with rich C vacancies by adding a few amounts of Ni single atoms during thermal treatment. Insightful investigation by various advanced characterizations is also carried out. It was revealed that the g-C<sub>3</sub>N<sub>4</sub> appears in the form of nanotubes. The additional Ni single atoms play a key role on the formation of C vacancies and amine groups during post-thermal-triggering treatment. The defects could also induce microporous structure, resulting in high surface area of 73 m<sup>2</sup>/g. In addition, the emergent carbon defects shift the conduction band of g-C<sub>3</sub>N<sub>4</sub> to a higher energy level, which is beneficial for increasing reduction ability. Meanwhile, the exposed edge amino moieties enhance CO<sub>2</sub> adsorption ability, verifying by experimental and theoretical simulation results. The amine-functionalized g-C<sub>3</sub>N<sub>4</sub> nanotubes with optimum loading of Ni single atoms (5Ni/CN) exhibit superior visible-light-induced CO<sub>2</sub>-to-CO conversion rate of 232.9 μmol g<sup>-1</sup>h<sup>-1</sup>, which is 66 and 3 times higher than those of bulk g-C<sub>3</sub>N<sub>4</sub> (4.9 μmol g<sup>-1</sup>h<sup>-1</sup>) and pure g-C<sub>3</sub>N<sub>4</sub> (123.0 μmol g<sup>-1</sup>h<sup>-1</sup>), respectively. This work is first reported on new insights into the synthesis of amine functional groups-modified g-C<sub>3</sub>N<sub>4</sub> with a unique structure for effective photocatalytic CO<sub>2</sub> reduction.

**Keywords:** g-C<sub>3</sub>N<sub>4</sub> nanotubes, carbon vacancies, Ni single atom, CO<sub>2</sub> photoreduction, visible light irradiation

# Copper-nickel alloy modified silicon photoanodes for photoelectrochemical water oxidation and urea oxidation

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## Abstract

The development of silicon (Si) photoanodes for photoelectrochemical (PEC) oxidation is very crucial for the progress of solar-driven hydrogen production. Apart from the typical water oxidation reaction or oxygen evolution reaction (OER), the urea oxidation reaction (UOR) is gaining more attention recently as it requires less energy input and can be applied as urine or urea-based waste management. Inhomogeneous metal-insulator-semiconductor (MIS) Si photoanodes prepared via cathodic electrodeposition have been utilized for PEC water oxidation with good performance and stability. However, there is very little development on electrodeposited metal co-catalysts for UOR on Si photoanodes. In this work, we study electrodeposited copper-nickel (CuNi) alloy-modified Si photoanodes for PEC water oxidation and urea oxidation. The optimized Si photoanodes for OER exhibit a low onset potential of 1.15 V<sub>RHE</sub> [V vs. reversible hydrogen electrode (RHE)] and a current density of 6 mA cm<sup>-2</sup> at 1.23 V<sub>RHE</sub> (water oxidation potential). The stability of the photoanodes in 1 M KOH is around 1.5 to 5 h and can be extended to 15 to 40 h in a K-borate/Li-borate buffer. We observe that the electrode activation process by potential cycling is essential to obtain high performance photoanodes. Further, CuNi alloy-modified Si photoanodes are tested for UOR. The optimized photoanodes are able to drive UOR at a lower onset potential (1.05 V<sub>RHE</sub>) when compared to that with OER and generate a current density of 31 mA cm<sup>-2</sup> at 1.23 V<sub>RHE</sub>. Importantly, CuNi alloy can prolong the stability for UOR on Si photoanodes when compared to a Ni film deposited by a vacuum-based process. Moreover, our electrocatalytic study indicates that CuNi alloy shows higher activity toward UOR than pure Ni metal. This work demonstrates that metal alloys can further improve the properties of inhomogeneous MIS Si photoanodes which can be efficiently utilized for both OER and UOR.

**Keywords:** Photoelectrochemical water splitting, Silicon photoanodes, Urea oxidation, Copper-nickel alloy, Electrodeposition

# Accelerated Synthesis of Nanolayered MWW Zeolite by Interzeolite Transformation

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## Abstract

Hierarchically organized zeolites offer substantial benefits over conventional bulk zeolites in both conventional and emerging catalytic processes.<sup>[1]</sup> However, the synthesis of such advanced structured zeolites is typically lengthy (> 7 days) and requires complex organic templates or several sequential steps, eventually preventing their applications on a practical scale.<sup>[2]</sup> Herein, the accelerated synthesis of nanolayered MWW zeolite has been developed by combining the interzeolite transformation (IZT) and dual-templating strategies. Cheap precursors, including FAU zeolite, hexamethylenimine (HMI), and cetyltrimethylammonium bromide (CTAB) were employed respectively as Al source, structure directing agent, and exfoliating agent. Colloidal silica was used as the main source of Si. By comparing a conventional synthesis of nanolayered MWW using amorphous precursors at a similar Si/Al ratio of 12.5, the IZT approach offered a reduction of synthesis time from 168 h to 48-72 h. Tracking the changes of structural, textural, morphological, and chemical properties during crystallization indicates that 4-membered ring building units (4MR) from FAU play an important role in the rapid formation of MWW, while CTAB reduces MWW growth in the c-direction. Consequently, these phenomena show the merits of the transfer of specific ring-building units in the synthesis of conventional bulk zeolite via IZT<sup>[3-4]</sup> and *in situ* exfoliation to separate MWW nanolayers in the conventional synthesis nanolayered via amorphous precursors.<sup>[5]</sup> Besides nanolayered MWW synthesis, lowering the Si/Al of the synthesis gel from 12.5 to 7.5 can also afford nanolayered FER zeolite after 72 h. The benefits of nanolayered MWW zeolite were shown in the improved catalytic performance in Diels-Alder Cycloaddition (DAC) reactions of 2,5-dimethylfuran and ethylene, a promising route to obtain biobased p-xylene due to the enhanced external surface area and increased accessibility of strong Brønsted acid sites.

**Keywords:** Zeolite, Synthesis, Interzeolite transformation, Nanolayer, MWW

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# Accelerated synthesis of hierarchical FER nanoneedles via ETL seed-assisted approach and their application in bioethanol dehydration

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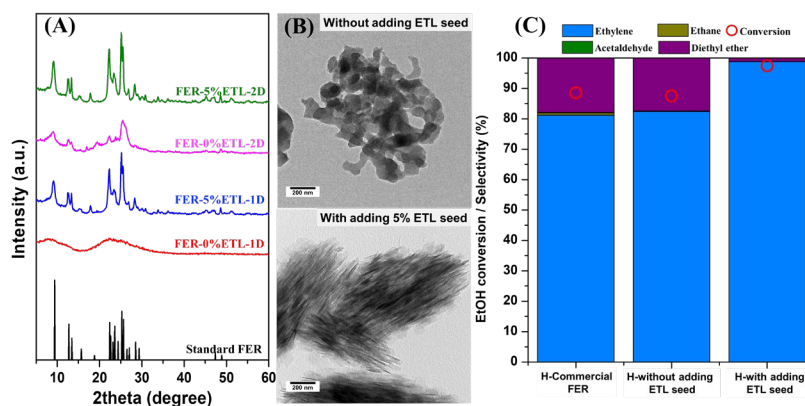
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## Abstract

The rational design of zeolite nanostructures in a molecular level is one of the interesting aspects because it allows to produce a highly efficient catalyst applied in various reactions. However, it often suffers from some drawbacks because most synthesis approaches require complex procedures and time-consuming processes. To overcome this problem, the development of a new synthesis approach with the combination of one-pot and speeding-up synthesis approaches would be one of the promising research topics. In this contribution, the rapid synthesis of hierarchical ferrierite nanoneedles has been demonstrated using chlorine chloride as a structure-directing agent and sodium cations ( $\text{Na}^+$ ) as the mineralizing agent via the ETL seed-assisted approach in a hydrothermal process. Interestingly, by adding a small amount of ETL seed, the crystallization growth could be accelerated and the FER framework can be directly formed due to the aid of the similar building units (CBUs), namely *mor*, which is the main units of both FER and ETL zeolites. In contrast, no crystalline phase could be formed without adding ETL seed at the early stage of synthesis. The literally different morphologies between ones obtained by without and with adding ETL seed were observed. The bulk and irregular shape was obtained without adding ETL seed, while the nanoneedles shape was obtained with adding ETL seed. In addition, the use of other zeolite frameworks as seeds in hierarchical FER nanoneedle synthesis has been investigated. It was found that *mor* CBUs play an important role in FER formation. Finally, the bioethanol dehydration reaction has been performed to illustrate the beneficial aspect of synthesized hierarchical FER nanoneedles in catalysis.

**Keywords:** zeolite synthesis, hierarchical zeolite, seed-assisted approach, bioethanol dehydration



**Figure 1.** Illustration of (A) the measured PXRD pattern of synthesized Hie-FER without and with adding ETL seed (B) TEM images of synthesized Hie-FER without and with adding ETL seed, and (C) Catalytic performance in bioethanol dehydration at 300 °C for 24 h (WSHV 5 h<sup>-1</sup>) over H-commercial FER, H-Hie-FER without and with adding ETL seed

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## A New Electrode Using a Cu-SiO<sub>2</sub> nanocatalyst for Reducing Chloride Ions from Eshidiya Mine Wastewater, South Jordan

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### Abstract

Jordan faces a substantial water scarcity issue compared to many other countries worldwide. The Eshidiya mine, specifically, utilized a considerable volume of fresh water for processing rock phosphate. This process resulted in the discharge of wastewater with elevated chloride ion levels, leading to the pollution of local surface water, groundwater, and soil. Cu-SiO<sub>2</sub> nanoparticles were created to decrease the Cl<sup>-</sup> concentration in wastewater from the Eshidiya mine. The Brunauer-Emmet-Teller (BET) analysis indicated that the Cu-SiO<sub>2</sub> nanoparticles possessed a surface area of 470.7309 cm<sup>2</sup>/g and a pore volume of 0.296093 cm<sup>3</sup>/g. Through Cyclic Voltammetry (CV) analysis, it was observed that the chloride ions exhibited a slight reduction of 0.11 V in the anodic peak, accompanied by a corresponding current density of 5.8 mA/cm<sup>2</sup>. Linear Sweep Voltammetry (LSV) reveals the best scanning rate of 0.05 V/s for chloride ion detection. Differential Pulse Voltammetry (DPV) demonstrates two clear peaks at 0.127 V and 0.183 V, with corresponding currents of 4.36x10<sup>-8</sup> and 3.24x10<sup>-8</sup> A. The i-t curve indicates the electrode achieves equilibrium activity, needing revival by reversing voltage from 0.71 volts to -0.71 volts.

*Keywords: Mine wastewater, Nano catalyst, Chloride reduction, Electrochemical techniques*

## Zinc-organic framework and titanium dioxide nanocomposite for use as photocatalyst for dye degradation

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### Abstract

This research aims to fabricate new composite photocatalyst materials between a new zinc-organic framework and titanium dioxide nanoparticles. The first step was a synthesis of a new zinc-organic framework using microwave method. The zinc-organic framework contained the central atom of one zinc ion coordinated by two molecules of 4,4'-Bipyridine ligands and two molecules of succinic acid ligands to form zinc-organic framework complexes,  $[Zn(4,4'-bipy)_2(Suc)]_n$  (MOF). The second step was synthesizing new composite materials by formulating  $TiO_2$  nanoparticles on the surface of MOF crystals via three different methods. The first method was synthesized by co-precipitating  $TiO_2$  powder distilled in MOF solution and then microwave heating at 800 W for 10 minutes (MOF\_C1). The second and third methods were synthesized by co-precipitating of MOF after microwave heating together with  $TiO_2$  solution (MOF\_C2) or  $TiO_2$  powder (MOF\_C3) respectively. SEM images revealed  $TiO_2$  nanorods were well deposited on entire MOF surface. The X-ray diffraction (XRD) results showed that the composite materials comprised a small amount of  $TiO_2$  anatase crystal structure and the majority of MOF. Finally, the methyl orange dye degradation process was used to study the as-synthesized catalyst efficiency. A 100 mg catalyst loading was immersed in 100 ml of 2.5 mg/L of methyl orange dye solution under UV-C light irradiation for 300 minutes. The dye degradation efficiency of MOF, MOF\_C1, MOF\_C2, and MOF\_C3 were 24.56%, 46.77% and 37.64% respectively.

*Keywords: Metal-Organic framework, Composite material, Titanium dioxide, Photocatalytic, Dye degradation*

## Antibacterial Effect of Core-Shell Gold-Based Nanoparticles in Paint

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### Abstract

Nanoparticles have emerged as a promising solution to enhance antibacterial properties, create hygienic surfaces, and extend shelf life of water-based paints and coatings. However, the bacteria and other microbes develop themselves as multidrug-resistance microbes. Furthermore, the development of bacteria against silver nanoparticles has recently been reported. Therefore, it is important to develop new agents against these bacteria. This study provides a new form of nanoparticles called core-shell gold-based nanoparticles (CGNPs) to solve this problem. The CGNPs were then added to the water-based paint. After forming a paint film, the antibacterial activity was investigated by testing Gram-negative drug-resistance bacteria, *Escherichia coli* BAA-1161. The test was performed according to the JIS Z 2801/ISO 22196 protocol at different contact times (0 and 24 h). The antibacterial activity of unwashed and washed paint films was also compared. The characterization of the CGNPs in the paint films was included. Overall, we found that the CGNPs had the ability to inhibit the growth of bacteria in the paint films.

**Keywords:** Core-shell gold-based nanoparticles, Antibacterial activity, Drug-resistance bacteria, Paint

# Cellulose Benzenesulfonic Acid as a Solid Acid Catalyst for Fructose Conversion to 5-HMF

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## Abstract

Cellulose benzenesulfonic acid (CBSA) was successfully synthesized by reacting cellulose microcrystal (CMC) with 4-chlorobenzenesulfonic acid in toluene. The CBSA product was characterized by FTIR, PXRD, TGA, and Sulfur analysis. The catalytic activity for fructose conversion to 5-HMF in DMSO of CBSA was examined and the effects of reaction temperature and reaction time on its activity were investigated. The results showed that CBSA of 10 wt% loading exhibited the highest catalytic activity with the fructose conversion of 100% and 5-HMF yield of *ca.* 85% at the reaction temperature of 140 °C and the reaction time of 180 min. The recyclability of CBSA was studied and it was found that the activity dropped by approximately 29% and 89% after 2 and 3 reuse cycles, respectively.

**Keywords:** Cellulose benzenesulfonic acid (CBSA), 5-HMF, Biochemical, Biorefinery, Cellulose utilization



# Sustainable Production of Silver Doped Activated Carbon Using a Green Process: Facile Upscaling from Laboratory Scale to Pilot Plant

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## Abstract

Silver impregnated activated carbon (Ag/AC) is an effective material in various applications such as water treatment, drinking water purification, and air filtration process. Up to date, the production of the impregnation process of silver nanoparticles is regularly used a strong reducing agents and hazardous stabilizers, leading to environmental problems in wastewater. Recently, our research successfully developed a green method to produce Ag/AC in laboratory scale using biomass including glucose and tapioca starch. However, the limitations of laboratory scale are lack of real-world condition, and small sample size. To the best of our knowledge, Ag/AC product has never been reported for commercial manufacturing in Thailand, mostly import from abroad with a minimum order otherwise and it will be charged for shipping and fee. Thus, this work aims to produce Ag/AC in a pilot scale reactor using a green process. The results found that the characterizations of Ag/AC from pilot scale were similar to Ag/AC from laboratory scale such as morphology and size of silver nanoparticles, and surface area. The efficiencies of Ag/AC from pilot scale for removing gas and aqueous solutions forms such as volatile organic compounds (VOCs), and heavy metals were closely comparable with Ag/AC from laboratory scale. The silver release from Ag/AC in water treatment was lower than the standard of drinking water by WHO. Therefore, this pilot scale reactor can be used as guidelines technology to produce Ag/AC.

**Keywords:** Ag/AC, industrial pilot scale, adsorption process, volatile organic compounds (VOCs), disinfection, mercury removal

# Preparation of Mesoporous Nanosphere Carbon as an Efficient Heterogeneous Fenton-like Catalyst for Degradation of Reactive dyes

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## Abstract

The textile industry is one of the many industrial sectors in Thailand that produce dye-contaminated wastewater, which affects the environment and needs to be concerned. Developing composite catalysts with high removal efficiency and convenient separation is important for water treatment. This study synthesized Mesoporous Nanosphere Carbon (MC-700) for use to degrade reactive black-5 (RB-5) dye contaminated in water. The catalysts were prepared from the Stöber method with a Sol-gel polycondensation of resorcinol and formaldehyde to induce nanosphere shape and impregnated with iron oxides for magneto-responsive. Characterization results demonstrated that MC-700 contained Fe<sub>3</sub>O<sub>4</sub>, saturated magnetization of 16.01 emu/g, specific surface area of 277.18 m<sup>2</sup>/g, and mesopore volume of 0.45 cm<sup>3</sup>/g. Then, the obtained catalysts were examined by heterogeneous Fenton-catalyzed degradation of the RB-5 reaction. The result showed that MC-700 provided the tremendous maximum adsorption capacity of RB-5 (200.14 mg/g) and stimulated the decomposition of the H<sub>2</sub>O<sub>2</sub>, to enhance the generation of •OH radicals, which promoted oxidation of the dyes to realize 99.78% removal under 10 mM H<sub>2</sub>O<sub>2</sub> concentration, 1g/L catalyst, 400 ppm RB-5 initial concentration, and pH 3 at 30 °C. This study has shown that the Mesoporous Nanosphere Carbon exhibited good stability in repeated cycles, indicating that it could be reused as an effective catalyst in water treatment of organic pollutants.

*Keywords: mesoporous nanosphere carbon, Stöber method, azo dye, Fenton-catalyzed degradation.*

# Maximizing biodiesel production from waste cooking oil with KI/CaO/Al<sub>2</sub>O<sub>3</sub> catalyst using response surface methodology and artificial neural network application

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## Abstract

The process of producing biodiesel from waste cooking oil (WCO) involves going through a heterogeneous catalyzed transesterification technique. The potassium iodide/calcium oxide/alumina (KI/CaO/Al<sub>2</sub>O<sub>3</sub>) catalyst was prepared using the calcination and impregnation procedures. The novel catalyst was analyzed with X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy dispersive X-ray spectrometer (EDX). The significance of the three reaction parameters, such as the methanol to waste oil molar ratio, catalyst concentration, and reaction time, as well as their combined effect on biodiesel yield is explored through twenty of the pre-designed and completed experiments. Both the Box-Behnken design (BBD) based on response surface methodology (RSM) and the artificial neural network (ANN) based on artificial intelligence (AI) were utilized in order to optimize the process conditions and maximize the biodiesel production. For the purpose of predicting biodiesel yield, a quadratic regression model was developed and given a coefficient of determination (R<sup>2</sup>) value of 0.9886. At a molar ratio of 15:1 methanol to waste oil, with a concentration of 3.0 weight percent catalyst and a reaction period of 9 minutes, the maximum amount of biodiesel that can be produced is 98.37%. The findings of this study indicate that the BBD and ANN may be successfully applied to optimize and predict the maximum amount of biodiesel yield.

*Keywords: Optimization, Artificial intelligence, Biodiesel production, Clean energy technology, Catalysis for bioenergy*

## Kinetic study of converting fructose into 5-HMF using sulfonated watermelon rind biochar as acidic heterogeneous catalyst in aqueous media solvent

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### Abstract

Nowadays, biorefinery is an alternative way to convert depletion of fossils to renewable resources. Biomass consists of cellulosic contents applied to produce value platform chemicals, i.e., 5-hydroxymethylfurfural (5-HMF). The presence of acidic catalysts could accelerate dehydration of fructose to 5-HMF by donating protons owing to decreasing activation energy. From previous work, sulfonated watermelon rind biochar treated with sulfuric acid concentration of 4.8 N (4.8WBS) was successfully grafted acidic functional groups on biochar and obtained fructose conversion of 72.3% and 5-HMF yield of 45.9% (reaction conditions: 0.2 g of catalyst, 40 w/v% of fructose, 30 mL of DI water, temperature of 160 °C, 90 min). It was implied that 4.8WBS could be advantageous to use as heterogeneous catalyst for conversion of fructose to 5-HMF. Effects of dehydration conditions such as time and temperature significantly influenced the conversion of fructose and yield of 5-HMF. Herein, this work will investigate kinetic parameters including rate constant and activation energy comparing absence with presence of catalyst. To conduct an accurate experiment, dehydration reactions were performed in hydrothermal reactor using sulfonated watermelon rind biochar (4.8WBS) at temperature ranges of 150 to 180°C within 120 mins. Liquid products will be filtered by a syringe filter diameter of 0.2 µm and analyzed by High-performance liquid chromatography (HPLC) with an Aminex sugar column. Kinetic studies on the effect of time and temperature on 5-HMF production from fructose will be deliberated and discussed.

*Keywords: biochar, watermelon rind, heterogeneous catalyst, 5-HMF, kinetic*

## Synthesis and characterization of mixed-metal azolate frameworks via post-synthetic process

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### Abstract

A mixed-metal approach in the synthesis of metal-organic frameworks (MOFs) is one of useful strategies to achieve a variety of desired properties or functionalities that may not be possible in a single-metal system. It involves incorporating two or more different metal ions into the framework structure. In this study, we synthesized mixed-metal azolate frameworks and conducted a comparative analysis of their properties in relation to those of single-metal MOFs. Cu/Ni-trizole was obtained through a post-synthetic reaction, preserving the structure and morphology of the original Cu-trizole framework.

*Keywords: Metal organic frameworks, Metal exchange*

# Conjugated Polymers Immobilized by Matrix for Photocatalytic Hydrogen Production

Yu-En Sun<sup>a</sup>, Wei-Cheng Lina, Rou-Han Lai<sup>a</sup>, Tse-Fu Huang<sup>a</sup>, Li-Yu Ting<sup>a</sup>, Yuan-Ting Tseng<sup>a</sup>, Yi-Hsiang Wu<sup>a</sup>, Ying-Rang Zhuang<sup>a</sup>, Bing-Heng Li<sup>a</sup>, Ho-Hsiu Chou<sup>a,b,\*</sup>

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## Abstract

Solar hydrogen production via photocatalytic water splitting is a highly investigated area of research worldwide, driven by its tremendous potential for harnessing solar energy and addressing climate-related concerns. Conventionally, water-splitting photocatalysts are utilized as suspended powders. However, their tendency to sediment poses a significant challenge in terms of large-area processing compatibility. Additionally, existing thin film approaches relying on delicate glass substrates introduce complexity to future device applications. To address these limitations, we present a novel system design providing a simplified and scalable solution. The approach involves the use of immobilized conjugated materials with exceptional stretchability and free-standing properties. Notably, we introduce poly(propylene glycol), tolylene 2,4-diisocyanate terminated (PTD), as a substitute for traditional substrates in thin film hydrogen production tests. By physically blending the organic photocatalysts into the PTD structure, the detachment of photocatalysts during the photocatalytic hydrogen evolution process is effectively prevented. This research aims to establish a universal strategy applicable to various kinds of polymers, including soluble and insoluble conjugated polymers with different absorption ranges. The results showcase a promising hydrogen evolution rate of 23.36 mmol g<sup>-1</sup>h<sup>-1</sup>, significantly outperforming traditional thin film processes for all types of conjugated polymers. Moreover, the ability to tune the film thickness enables precise control and enhancement of the light absorption area. Implementing this pioneering approach holds the potential to enhance the efficiency, stability, and durability of photocatalytic water splitting, thereby paving the way for practical large-scale solar hydrogen production.

*Keywords: Photocatalysts, water-splitting, stretchability, thin film*

## Translating electrochemical biosensor technologies from the university environment into the commercial space

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<sup>a</sup>*Centre for Advanced Measurement Science and Health Translation, University of Strathclyde, Glasgow, UK.*

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### Abstract

Since 2021 two spin out companies have emerged from my laboratory, one looking at detection of antibiotic susceptibility in urinary tract infection samples in under one hour (Microplate Dx) and the other developing a low-cost electrochemical detection platform aimed at measuring a range of important biomarkers at the point of care. This talk will summarise my experiences from launching these two innovative high startups and cover areas such as: intellectual property protection, raising venture capital, establishing a company and its culture and adapting from academic research for the commercial environment. In addition to company formation the group is active in other knowledge exchange areas such as setting up a national research Centre with industrial partners, specific knowledge exchange projects with diagnostics companies and making IP licensing deals with diagnostics companies. Again, aspects of these activities will be covered to give a full picture of our experience gained from translating projects from the University into real world use.

*Keywords: electrochemical biosensors, commercialization, venture capital, intellectual property*

# HEOLE: Organic Solar Sails and Textiles for Marine Decarbonation and Building Integrated Photovoltaic

Guillaume Wantz<sup>a,\*</sup>

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## Abstract

This presentation is about the start-up company HEOLE, created in 2021. HEOLE is a developer of flexible photovoltaic solar solutions embedding organic photovoltaic modules (OPV). OPV solar is an emerging photovoltaic technology with unique properties. They are printed on large scale, potentially at low cost. They are light weight, flexible and semitransparent. They show a very low carbon footprint and short energy payback times. With all these promises, Héole is integrating OPV modules in first-of-their-kind products starting with sails for sailboats. Indeed, Héole has showed the first OPV solar sail in May 2022 and others lately. Such sail enable to produce all the electricity needed for onboard usage. The sail remains fonctionnal, flexible and robust. The ultimate goal of such sail is to provide enough energy to power electric engine, thus pushing marine decarbonisation. Héole has also demonstrated in 2023 some building integrated systems combined with vegetalisation of roofs (green roofing solar PV). Héole is planning to launch a solar zeppelin in 2025. Such a flying vessel will be autonomous, fossil-fuel free and able to fly non stop. This presentation will focuss on these developments and also showing experimental results obtained on commercially available OPV modules.





**Short Bio:**

Guillaume Wantz graduated from the School of Chemistry and Physics of Bordeaux (ENSCPB) in 2001 including a thesis work at Philips Research (Eindhoven, NL) on ink-jet printing. He received his Ph.D. in Electronics Engineering from the University of Bordeaux in 2004 working on Polymer Light Emitting Diodes. He was Assistant Professor at the University of Bordeaux working on Organic Field Effect Transistors with research stays at Queen's University (Kingston, Canada). In 2006, he was appointed as tenure Associate Professor at the Bordeaux Institute of Technology (Bordeaux INP). He is Professeur des Universités since 2021. His research interest is on Organic Electronics with a focus on polymer photovoltaic solar cells (OPV). He was invited-professor at Queen's University (Kingston, Ontario, Canada) in Spring 2012 and at Univ. of Massachusetts (Amherst, USA) in Fall 2014. He has been appointed at the "Institut Universitaire de France" (IUF Paris) in 2016. Since 2017, he is Associate Editor for the journal "Materials Chemistry Frontiers" (RSC). He is co-founder of Héole, a company developing flexible OPV products including solar-powered sails for yachting, a solar zeppelin and some BIPV flexible OPV products. To date, he has published 125 research papers in peer-reviewed international journals and issued 7 patents (h = 37 – 6000 citations – source Google Scholar).

Guillaume Wantz  
Professeur des Universités  
Member of Institut Universitaire de France (IUF)  
Head of CNRS network on Organic and Hybrid Photovoltaic  
Associate Editor "Materials Chemistry Frontiers" (RSC)

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## Digital Temperature Indicator (DTIs) – Battery-free Smart Label based on Thermoresponsive Materials

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<sup>a</sup>*Cleantech and Beyond Co., Ltd., Rayong, Thailand*

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### Abstract

The inefficient supply chain, lack of temperature control, and mismanagement of expiry dates are major contributors to food and pharmaceutical waste. This problem results in the yearly discarding of 1.3 billion tons of food and \$750 billion worth of medications. These numbers not only represent significant financial losses but also the wastage of valuable resources. Therefore, it is crucial to have the ability to track temperature excursions of goods, especially at the item level. However, the current technologies available in the market are lacking in some aspects. Active data loggers require batteries, while analogue indicators lack a digital interface.

Cleantech & Beyond offers a new solution called Digital Temperature Indicators (DTIs), which is the first technology to combine three important features: battery-free operation, a wireless digital interface via standard RFID/NFC communication, and data-logging capability. The DTIs are constructed using our patented, specially formulated, thermoresponsive materials. They can track and log temperature excursion events at the item level without the need for any external power sources. The data can be read through standard RFID/NFC equipment, allowing seamless integration into existing logistics and inventory infrastructure. By ensuring that products are shipped, stored, and used at safe temperatures, the DTIs can improve operational efficiency, sustainability, and build stronger customer trust.

*Keywords: Temperature indicator, Smart label, Battery-free, NFC, RFID*

# Pimpisut Worakajit

## General Manager

### SUMMARY

Results-driven multidisciplinary engineer with expertise in advanced materials characterization and electronic device fabrication. Strong coordination and project management skills ensure seamless execution from start to finish. Detail-oriented with a passion for leveraging cutting-edge technologies to drive innovation. Committed to delivering exceptional results and contributing to technological advancements.

### EXPERIENCES

#### General Manager 2023-Present

Cleantech and Beyond Co., Ltd.

Cleantech and Beyond is a deep tech startup that specializes in development advance materials for environmental sensing applications.

- Oversee day-to-day operations.
- Financial management
- Evaluate and improve operation and financial performance.
- Ensure employee work productively and develop professionally.
- Provide solution for issues.

#### Project Manager 2021-2023

Government-funded Project

The project was funded by Program Management unit for Competitiveness (PMUC), Vidyasirimedhi Institute of Science and Technology (VISTEC) and IRPC Public Company Limited to develop a high-TRL Temperature Indicator and scale up production for commercialization.

- Coordinate people and process to ensure that the projects are delivered on time and produce the desired results.
- Financial management
- Provide solution for issues

#### Researcher 2020-2021

EDM - IRPC collaboration project

This project aims to develop a novel functional material for sensing applications.

- Create research plan.
- Experimental design
- Provide solution for issues.

#### Lab Manager 2016-2019

Electronic Device & Materials Innovation Laboratory (EDM)

EDM Lab is a member of Materials Science and Engineering department, VISTEC.

- Oversee the operations of various types of labs to ensure that safety protocols are followed and all equipment is supplied and maintained.
- Financial management and purchase requisition.

### EDUCATIONS

#### Ph.D. in Materials Science and Engineering 2015-2023

Vidyasirimedhi Institute of Science and Technology

#### Bachelor's in engineering (Biomedical Engineering) 2011-2015

Mahidol University



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### SKILLS

- Leadership
- Management
- Communication
- Problem solving
- Teamwork
- Adaptability
- Critical Thinking
- Negotiation

### LANGUAGES

- Thai
- Eng

# Challenging Factors in Advancing Research to Business; Case Studies

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## Abstract

Bringing a work from laboratory research toward a new business has been challenging disregard type of business. Typically, technical feasibility of research projects has been demonstrated by their functional prototypes at Technology Readiness Level 4 (TRL 4). These results often bring attentions under expectation of solving specific pain points leading to great opportunity for future business. The next question should be asked “How might we bring research from TRL4 toward TRL9 and to new business?” The answers are not simple and often time seems to be difficult considering numerous factoring beyond technological aspects. Herein, the technological and non-technological challenges during TRLs progression will be discussed. The relationship between the technology readiness levels and the business readiness levels will be off the focus as one of the key success factors. Some case studies are considered as examples to better visualize the challenges arising from each case.

*Keywords: Technology readiness levels, business readiness levels*

**Short Bio: Dr. Chuchawin Changtong**



ตำแหน่งและสังกัด: ผู้อำนวยการ หน่วยวิจัยและพัฒนาวัสดุนาโน (IRPC Innovation Center)

ความเชี่ยวชาญ: วัสดุนาโนคอมโพสิต สำหรับอุปกรณ์อิเล็กทรอนิกส์ และวัสดุกักเก็บพลังงาน

การศึกษา: Ph.D. in Chemistry (Worcester Polytechnic Institute, MA USA)

**ผลงานการพัฒนางานวิจัยเชิงพาณิชย์**

Changtong C., Carney D.W., Luo L., Zoto C.A., Lombardi J. L., Connors R. E. “A porphyrin molecule that generates, traps, stores, and releases singlet oxygen” J. Photochem. and Photobio. A: Chem. 2013, 260, 9– 13.

Lombardi, J. L.; Changtong, C. “Chemically-resistant coating composition” U.S. Pat. 8481446B2, 2013.

Connors R. E.; Changtong, C. and Lombardi J. L. “Porphyrin compounds comprising one or more pyridone moieties” U.S. Pat. 8445683, 2013.

Lombardi, J. L.; Changtong, C. “Fabrics comprising a photocatalyst to produce singlet oxygen from ambient oxygen” U.S. Pat. 8921243B2, 2014.

**ประสบการณ์การทำงานที่เกี่ยวข้อง**

การพัฒนากระบวนการสังเคราะห์โพลิเมอร์นำไฟฟ้าในระดับโรงงานต้นแบบ (pilot production)

การพัฒนากระบวนการปรับปรุงพื้นผิวของวัสดุนาโนคาร์บอนในระดับโรงงานต้นแบบ (pilot production)

การพัฒนาหมึกนำไฟฟ้า เพื่อนำไปใช้ทำขั้วนำไฟฟ้าชนิดฟิล์มบาง ด้วยกระบวนการพิมพ์ระดับ

อุตสาหกรรม

การพัฒนาหมึกนำไฟฟ้า เพื่อนำไปใช้สำหรับเสาอากาศของอุปกรณ์ RFID ด้วยกระบวนการพิมพ์ระดับ

อุตสาหกรรม

การพัฒนาวัสดุนาโนคอมโพสิตเพื่อใช้สำหรับขั้วคาโทด ของแบตเตอรี่ ลิเทียม ซัลเฟอร์

การพัฒนาวัสดุนาโนคอมโพสิตเพื่อใช้สำหรับอุปกรณ์ซูเปอร์คาปาซิเตอร์

# Application of X-Ray Absorption Spectroscopy at TPS 44A1 Beamline to Decipher the Active Site in Energy Material Science

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## Abstract

X-ray absorption spectroscopy (XAS), which includes X-ray absorption near edge structure (XANES) and extended X-ray absorption fine structure (EXAFS), is a powerful tool at synchrotron radiation facilities. The XANES region of XAS provides the electronic structure and local geometric information, and the EXAFS region is used to obtain the detailed local atomic structure around the absorbing atoms, such as the nearest neighbor atomic type, the number of atoms in a specific coordination shell, the interatomic distance, and the structural disorder. Generally, one full spectrum which includes EXAFS region needs to spend 15 to 40 minutes collecting. Unfortunately, most chemical reactions happened in a few seconds. Therefore, it is urgent to collect one full spectrum in a few seconds. Here, a quick-scanning X-ray absorption spectroscopy beamline (TPS 44A1) at the Taiwan Photon Source, is presented. The beamline is equipped with a quick-scanning monochromator (Q-mono), which can provide conventional step-by-step scans and on-the-fly scans for a full spectrum.

Fossil fuels are the most commonly used fuels for energy in our daily lives. However, the concentration of carbon dioxide in the atmosphere has increased year by year due to the excessive use of fossil fuels. In turn, it has caused extreme changes in the global climate. Therefore, finding low-carbon emissions and clean renewable energy is the goal of all countries in the world. Hydrogen is regarded as an ideal alternative clean fuel because it can be effectively converted into energy without producing harmful substances or greenhouse gases. It can be produced by thermally cracking hydrocarbons to produce hydrogen or using photocatalytic or electrocatalytic ways for water splitting. These catalytic reactions are extremely dependent on the activity of metal catalysts. Therefore, it will become an important key to the promotion of hydrogen fuel if the activity of catalysts can be improved and its cost can be reduced. However, it is very important to understand the working pathways of the catalyst. Here, *in-situ/operando* electrocatalyst characterization and methane pyrolysis reactions were presented by XAS technique.

*Keywords: Time-resolved XAS, HER, OER, Methane pyrolysis*

**Short Bio: Jeng-Lung Chen**

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**Biographical Information:**

Spokesperson, Taiwan Light Source Beam Line 17C, National Synchrotron Radiation Research Center, Taiwan (2023~Now)

Manager, Taiwan Photon Source Beam Line 44A1, National Synchrotron Radiation Research Center, Taiwan (2019~Now).

Assistant Research Scientist, National Synchrotron Radiation Research Center, Taiwan (2015~Now).

Postdoctoral Fellow, National Synchrotron Radiation Research Center, Taiwan (2012~2015).

PhD in Physics, Department of Physics, Tamkang University, Taiwan (2005-2012)

Exchange Student, Advanced Light Source, Lawrence Berkeley National Laboratory, California, USA (2008~2010).

**Research Interests:**

In-situ/operando X-ray Absorption Spectroscopy.

X-ray Fluorescence Microscopy.

**Publications:**

For the complete list, please go to the following link.

[https://scholar.google.com.tw/citations?hl=zh-TW&user=Ns4CkBoAAAAJ&view\\_op=list\\_works&sortby=pubdate](https://scholar.google.com.tw/citations?hl=zh-TW&user=Ns4CkBoAAAAJ&view_op=list_works&sortby=pubdate)

# NanoRaman: Integrating AFM and Raman to Provide Colocalized and Tip-Enhanced Analysis

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## Abstract

Atomic force microscopy (AFM) has made nanoscale imaging an affordable reality. The technique provides a continuously growing variety of surface analysis methods for the physical characterization of materials. Raman spectroscopy has long provided a versatile way to determine the structure and chemical composition of molecules. In combination, the two techniques yield an attractive and unique tool for entering the nano-world. With HORIBA versatile platform, colocalized AFM-Raman measurement and tip-enhanced Raman spectroscopy (TERS) are powerful and reliable techniques for studying samples at nm scale. Colocalized AFM-Raman measurement is the sequential or simultaneous acquisition of correlated AFM and Raman maps. AFM provides topographic, mechanical, thermal, electrical, and magnetic properties, on the other hand confocal Raman spectroscopy and imaging provides specific chemical information about the material. TERS utilizes surface plasmonic effect and generates hot spot at the probe tip. The field extends only for a few nanometers from the tip surface. Bringing the hot spot close to the sample significantly enhances the Raman signal, often by a power of  $10^5$  or  $10^6$ . NanoRaman now has been used in different research fields, from materials science to life science.



**Short Bio: Che Boyang, Ph.D.**

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**Education**

Nanyang Technological University, Singapore Aug 2014 - Jun 2019  
Ph.D. in Interdisciplinary Graduate Program, Materials Science and Engineering  
Thesis: Conjugated polymer-based composites for electrochromic applications  
GPA: 4.75/5.0

Nanyang Technological University, Singapore Aug 2010 - Jun 2014  
B. Eng. in Materials Science and Engineering  
GPA: 4.55/5.0

- MOE SM2 scholar
- Dean's List student 2010/2011

Aalto University, Finland Aug 2012 - Dec 2012  
Exchange program in School of Chemical Technology

**Professional Experience**

**HORIBA Instruments (Singapore) Pte Ltd**

Application Scientist  
Mar 2022 - Present

- Compiled, archived & provided effective sales tools, technical support, and training to distributors and regional sales team to support their selling role.
- Stayed abreast with in-depth knowledge of the current and future market trends, including technology trends, customer applications and competitive technology, as relates to the tasked product lines, including Raman, AFM, fluorescence, ellipsometer, OSD, etc.
- Assisted the regional sales team in new application development according to emerging market opportunities and requirements in the region.
- Developed new market opportunities as well as supported growth in emerging markets by maintaining and developing relationship with universities, research Institutes, governmental agencies, industry and distributors, key customers, potential customers, and key opinion leaders in related community.
- Provided recommendation, coordination and planning of a range of regional marketing activities including attendance at tradeshow, seminars, product launches and regular product specific mail-outs with the Regional Marketing Team.
- Became the subject-matter expert and advised customers on experiment design, sample preparation, data analysis, etc.
- Assisted the Service Team by providing technical/application support with installations, validations and troubleshooting problems for customers.
- Maintained in-house equipment in good working condition and troubleshoot problems to ensure uninterrupted service.

# Tip-Enhanced Raman Scattering for Nanoscale Investigation

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## Abstract

Tip-enhanced Raman scattering (TERS) is a method integrating the benefits of surface-enhanced Raman scattering (SERS) with scanning probe microscopy (SPM). SERS allows the collection of Raman spectra of minute quantities of molecules adsorbed onto rough metal surfaces or nanoparticles. On the other hand, SPM techniques such as atomic force microscopy (AFM) and scanning tunneling microscopy (STM) can determine nanoscale topologies in samples. Because of this, TERS combines the best parts of both methods to provide molecular information about very small samples in specific nanoscale areas. Herein, three cases of TERS applications are presented. The first focus involves examining the structural changes of graphene oxide (GO) within the context of silver/graphene oxide (AGO) nanocomposites. The decoration of GO by AgNPs also affects the properties of GO. Hence, acquiring comprehensive knowledge on the interactions between GO and AgNPs would provide valuable insights for the manipulation and regulation of the features of nanocomposites. Second, a TERS tip was chemically modified with pH-sensitive molecules. The local pH in the nanoregion can be determined with a spatial resolution of ~400 nm. The pH value obtained from the measurement becomes the pH of the bulk solution when the distance between the tip and the surface is approximately 200 nm. This work proposes a potential method for pH sensing in aqueous biological samples. Third, a TERS tip was chemically modified with an achiral *para*-mercaptopyridine (*p*MPY) probe molecule to discriminate between two enantiomers. The presence of silver atoms at the apex of the tip in an asymmetric configuration results in the generation of an asymmetric electric field, leading to the tip acquiring chiral properties. When the asymmetric electric field is combined with changes in the charge-transfer (CT) states of the metal-achiral probe system, the Raman signals of the two enantiomers are enhanced in different ways.

**Keywords:** *tip-enhanced Raman scattering (TERS), silver/graphene oxide (AGO) nanocomposites, local pH, enantiomeric discrimination, chemically modified TERS tip*



**Short Bio: Prompong Pienpinijtham, Ph.D.**

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**Education**

2012                      Ph.D. (physical chemistry at Chulalongkorn University, THAILAND)  
2010–2011              Research student (with Prof. Yukihiro Ozaki at Kwansei Gakuin University, JAPAN)  
2007                      B.Sc. Degree (1<sup>st</sup> Class Honours in Chemistry at Chulalongkorn University, THAILAND)

**Scholarship & Awards**

2017                      Young Researcher Award from Chulalongkorn University, THAILAND  
2017                      Asahi Glass Foundation Overseas Research Grant, JAPAN  
2016                      Hitachi Research Fellowship, JAPAN  
2014                      Bronze medal from 42<sup>nd</sup> International Exhibition of Inventions of Geneva, SWITZERLAND  
2012                      Silver medal from 40<sup>th</sup> International Exhibition of Inventions of Geneva, SWITZERLAND  
2011                      Springer Poster Presentation Award at IUPAC International Congress on Analytical Sciences 2011, JAPAN  
2000–2012              The Development and Promotion of Science and Technology Talents (DPST) Project by Thai Government

**Areas of Research**

Molecular vibrational spectroscopy (IR and Raman spectroscopy)  
Design and fabrication of spectroscopic accessories  
Synthesis and characterizations of advanced functional precious metal (Ag, Au, Pt, and Pd) nanoparticles  
Surface- and tip-enhanced Raman spectroscopy (SERS and TERS)

**Working Experience**

2016–present           Assistant Professor at Department of Chemistry Faculty of Science, Chulalongkorn University, THAILAND  
2019 (June)            Visiting Assistant Professor at Jiangnan University, CHINA  
2018 (June)            Visiting Assistant Professor at Jiangnan University, CHINA  
2017 (July)            Visiting Assistant Professor at Kwansei Gakuin University, JAPAN  
2016–2017              Co-Research with Research and Development Center – Betagro Group, THAILAND  
2016 (June–Aug)      Visiting Assistant Professor at Kwansei Gakuin University, JAPAN  
2015–2016              Co-Research with IRPC Public Company Limited, THAILAND  
2015 (May–July)      Visiting Scientist at Kwansei Gakuin University, JAPAN  
2013–2016              Lecturer at Department of Chemistry Faculty of Science, Chulalongkorn University, THAILAND

## Quantum Electron Dose for Electron Beam Sensitive Nano-Materials

Tetsuo Oikawa<sup>a,\*</sup>, Hiroki Hashiguchi<sup>b</sup>, Yusuke Nishiyama<sup>b,c</sup>

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<sup>c</sup>RIKEN CLST-JEOL Collaboration Center, Tsurumi, Yokohama, Kanagawa 230-0045, Japan

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### Abstract

The transmission electron microscope (TEM) is the most powerful tool for obtaining morphological and structure information about materials; however, in the TEM, due to the strong beam irradiation (electron dose), some of the beam sensitive materials are broken while the TEM observation. Here, we proposed ultimately low electron irradiation of “quantum electron dose” technique. In the newly proposed technique, less than few electrons are dosed into the specimen, and the irradiation damage is reduced. One example of application is TEM imaging and electron diffraction (ED) for very sensitive L-histidine, combination with MDS (Minimum Dose System), TEM imaging and ED observation was performed at less than the critical dose of the L-histidine of 10 – 20 e-/nm<sup>2</sup>, thus the ED was obtained with quantum electron dose condition of 10 e-/nm<sup>2</sup>.

The second example is STEM imaging for very sensitive MFI zeolite; the STEM imaging was performed at 150 e-/Å<sup>2</sup>.

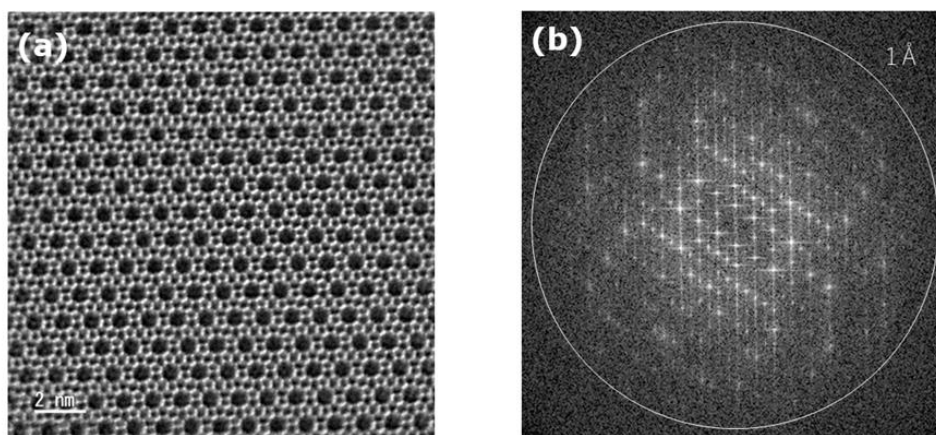


Fig.1 STEM image in quantum electron dose (150 e-/Å<sup>2</sup>) of MFI zeolite.

Owing to less electron damage on specimen, high-resolution crystal lattice image was obtained.

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**Keywords:** TEM, electron diffraction, MDS, critical dose, L-histidine

**Short Bio:**

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**Introduction:**

Dr. Tetsuo Oikawa is an internationally renowned expert in the field of electron microscopy, with a career spanning more than four decades of research and management experience. He has worked alongside some of the most respected academics and scientists, and his vast knowledge in electron microscopy, electron energy loss spectroscopy (EELS), analytical electron microscopy, and image science. Dr. Oikawa is currently a Senior Product Manager for TEM at JEOL Asia Pte. Ltd.

**Education and Job career**

1980 Graduated from Kogakuin University (Ph D Course)  
1980 Joined JEOL Ltd.  
2002 – 2012 Adjunct Professor of University of Sydney  
2005 – 2014 Invited Professor of University Paris Cite  
2012 - (Current) JEOL Asia Pte. Ltd.

Specialty: Electron microscopy, Analytical electron microscopy, Electron optics, Electron Energy Loss Spectroscopy (EELS), Image science.

# Nanoparticles in the Real World: Insights into Deposited Clusters from Aberration-Corrected Electron Microscopy

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## Abstract

Compared with the notional case of an isolated cluster (nanoparticle) at  $T=0$ , as addressed in some foundation theoretical treatments, two key factors will shape the behaviour of nanoclusters in the real world where we make experimental measurements. (i) The radiative environment (including the sample temperature and interaction with charged beams) and (ii) the material environment (including pressure/reactive gas and support). We will discuss four examples of the influence of these (coupled) factors; much of the work is unpublished.

(1) Aberration-corrected electron microscopy at variable elevated temperature probes the melting and isomeric energy differences of arrays of size-selected gold clusters bound to point defects on a carbon surface (while subject to irradiation by 200keV electrons) [1,2]. This is pre-Covid work forms a brief basis for the talk.

(2) Video imaging of a single deposited gold cluster on carbon at room temperature shows dynamic fluctuations between competing structures (isomers). Measurements at variable temperature enable equilibrium properties, branching ratios and relative barrier heights in the potential energy surface to be explored. The first such measurements will be reported.

(3) A study of 1 nm silver clusters (on carbon) compares clusters stored in vacuum versus those exposed to ambient before TEM. The work shows dramatic differences in the isomer proportions (fcc dominant versus Ih dominant), probably due to the effect of sulphur contaminants on the structural energetics [3].

(4) The role of the support is probed by studies of Au clusters assembled on carbon from sputtered gold atoms, where the transition from 2D to 3D morphology versus size appears to be delayed substantially compared with the free cluster. For Pt130 clusters on cerium oxide, the 2D versus 3D competition depends on which facet of ceria supports the cluster.

If time allows, I will briefly report progress on the scale-up of nanoparticle beam deposition towards the levels required for bespoke industrial manufacturing in vacuum. For example, implantation of lead clusters from the scaled-up MACS cluster beam into porous carbon creates an electrode architecture, illustrated by electrochemical generation of oxidising species for water treatment [4].

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**Short Bio: Prof. Richard E. Palmer**

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Richard is Head of the Nanomaterials Lab at Swansea University, UK, in his hometown, Swansea. He is also Professor, School of Physics, Nanjing University, China. His research on atomic clusters includes fundamental studies of atomic structure and dynamics as well as scale-up and applications in catalysis and biomedicine. Other well-established research themes include atomic manipulation in STM and semiconductor nanofabrication. He was awarded an MA and PhD at Cambridge where he also held 1851, Clare College and Royal Society Fellowships. At Birmingham he founded the UK's first centre for nanoscience. Honours include: IOP Boys Medal, Honorary Doctorate from Hasselt University, British Vacuum Council Yarwood Medal, EPSRC Senior Fellowship and Fellowships of IOP, RSC, Learned Society of Wales. He has 500 publications,  $h = 64$ ; including 20 families of patent applications. His work has led to a series of spin-out companies including Inanovate, Irresistible, Grove Nanomaterials, Nium. He is Editor-in-Chief of the journal *Advances in Physics: X* (Taylor and Francis) and Editor of the Elsevier Book Series 'Frontiers of Nanoscience'.

# Semiconducting Polymer Photocatalysts for Solar-driven Hydrogen Evolution

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## Abstract

By mimicking natural photosynthesis, artificial photosynthesis using polymer photocatalysts for the visible-light-driven generation of hydrogen through the splitting of water is an almost ideal process for the conversion of abundant solar energy into useable fuel in an environmentally friendly and high-energy-density manner. Photocatalytic hydrogen evolution through solar water splitting has received considerable attention due to an inexhaustible supply of solar energy. Extensive efforts have been made to prepare highly efficient photocatalytic materials. Appreciable amounts of organic semiconductors as photocatalysts have been specifically targeted to achieve outstanding photocatalytic activity because they have numerous attractive properties, including low-temperature processing, low-cost production, easily adjustable molecular structure, and tunable bandgaps that differentiate them from their inorganic counterparts. Since graphitic carbon nitride was successfully applied to photocatalytic hydrogen evolution systems in 2009, several types of research using polymeric photocatalysts, such as linear conjugated polymers, conjugated microporous polymers, polymer dots, covalent triazine frameworks, and covalent organic frameworks for hydrogen evolution have been gradually published. In a search for efficient photocatalysts that mimic such a function, here we will describe several series of newly designed polymers and polymer dots as photocatalysts for solar-driven hydrogen evolution from water. How to address the interface barrier between the polymer, water, and reagent will be included, to give a clear strategy for understanding the recent advances in this field.

**Keywords:** *Semiconducting Polymer, Photocatalysis, Solar-driven Hydrogen Evolution, Water-splitting*



## 3D-Image Analysis of the Microstructure of Porous High-Temperature Ceramics using FIB-SEM

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### Abstract

Recent advances in observation and evaluation techniques have made it possible to investigate the structure of materials on multiple scales, from nano to micro. In particular, the development and application of 3D (three-dimensional) observation in the microstructural analysis of materials is attracting attention. For instance, 3D image visualization techniques such as X-ray computed tomography (XCT) and magnetic resonance imaging (MRI) are widely used for biological materials. However, the resolution of these non-destructive tests is insufficient for some other types of materials. The physical properties of ceramic materials used under severe conditions such as high temperature and high pressure are greatly affected by raw materials, forming technique, sintering conditions, shape, size, and spatial distribution of defects remaining inside the materials. Particularly for porous high-temperature ceramics, the connectivity and tortuosity of the matrix and pores directly affect heat and fluid transport. Hence, it is important to acquire 3D images and accurately evaluate microstructures that can govern the physical properties. In this study, using porous high-temperature ceramics as a model material, we attempted to numerically assess the microstructure characteristics that affect the physical properties of ceramics by combining FIB-SEM and image analysis. The image processing, image analysis, and physical properties simulations were carried out using Fiji® and Avizo® software. The watershed phase segmentation method was applied to separate each phase to achieve artifact-free segmented phases. Quantifications of microstructural characteristics, namely volume fraction, domain size, centroid path tortuosity, fractal dimension, and degree of anisotropy, are presented. In addition, the permeability and electrical conductivity were simulated and correlated with the microstructural characteristics. This study suggests a direct correlation between pore size and permeability. As for electrical conductivity, a direct correlation between the volume fraction and connectivity was noticed.

*Keywords: high-temperature ceramics, FIB-SEM, image analysis, microstructure*

# The Influence of Polyvinylpyrrolidone on Dispersion Stability and Photocatalytic Activity of Ag-TiO<sub>2</sub> Nanoparticles with Ultra-Probe Sonication

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## Abstract

Silver-modified titanium dioxide nanoparticles (Ag-TiO<sub>2</sub> NPs) are well-known for water treatment and air purification; however, NP aggregation causes limited photocatalytic activity. Polyvinylpyrrolidone (PVP) is promising for the dispersion of NPs because of its sterically hindered effect. The concentrations of Ag-TiO<sub>2</sub> ranged from 0.1% m/v to 10.0% m/v, and the concentrations of PVP ranged from 0.006% m/v to 0.400% m/v were used for study. The concentrations of PVP at 0.006%, 0.050%, 0.200%, and 0.400% m/v mixed with the concentrations of Ag-TiO<sub>2</sub> at 0.1%, 1.0%, 5.0%, and 10.0% m/v presented the highest sedimentation height ratio and turbidity, which showed well-dispersed Ag-TiO<sub>2</sub> suspension. The effect of PVP showed a smaller average particle size and a narrower size distribution of Ag-TiO<sub>2</sub> with PVP than without PVP. The thickness of the PVP layer, approximately 2 nm, was covered on the surface of Ag-TiO<sub>2</sub> NPs investigated by high-resolution transmission electron microscopy (HRTEM). Fourier transform infrared spectroscopy (FTIR) was used to study the interaction forces between PVP and Ag-TiO<sub>2</sub> NPs on the surface. The chemical adsorption of PVP and Ag-TiO<sub>2</sub> NPs was demonstrated by the strong blue shift from 1648 to 1662 cm<sup>-1</sup> of the carbonyl group and the slightly blue shift from 1285 to 1288 cm<sup>-1</sup> of the nitrile group of the Ag-TiO<sub>2</sub>/PVP FT-IR spectrum. The photocatalytic activity degradation of methylene blue (MB) was used to study the performance of Ag-TiO<sub>2</sub>/PVP. Because the PVP layer coated on the surface of Ag-TiO<sub>2</sub>/PVP NPs provided a lower kinetic constant rate (5.06±0.76) ×10<sup>-3</sup> min<sup>-1</sup> than Ag-TiO<sub>2</sub> without PVP (9.90±0.74) ×10<sup>-3</sup> min<sup>-1</sup>, the kinetic rate constant of Ag-TiO<sub>2</sub>/PVP was still higher than that of commercial Ag-doped TiO<sub>2</sub> (3.21±0.77) ×10<sup>-3</sup> min<sup>-1</sup>.

**Keywords:** Silver-modified titanium dioxide, polyvinylpyrrolidone, dispersion stability, photocatalytic activity

## The Study of Nanoparticle Composition in Sub-urban area

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### Abstract

Thailand and other Asian countries are currently experiencing growing levels of air pollution. Particles or nanoparticles (NPs) in the atmosphere are an air pollutant that have a harmful impact on human health and the environment when exposed to excessive amounts. Little information is obtained by examining the composition of particles or nanoparticles. Understanding suitable health risk and impact assessment for health risk assessment in acute and chronic effects, as well as including the source of NPs in ambient air, are examples. As a result, this study investigated the chemical composition of NPs ( $PM_{0.1}$  and  $PM_{0.1-0.5}$ ) in rainy season by setting up the NPs sampling for ambient air using cascade air sample for size-classified particle at the rooftop of building of the Robotic Innovation and Automatic Mechanical Center, Thailand Institute of Scientific and Technological Research (TISTR), Technotani, Klongluang, Pathumtani province. The samples were collected after 48 hours to determine concentration levels, organic carbon (OC), and elemental carbon (EC) in  $PM_{0.1}$ ,  $PM_{0.1-0.5}$  particle sizes. The average concentration of  $PM_{0.1}$  was  $9.57 \mu\text{g}/\text{m}^3$ , whereas  $PM_{0.1-0.5}$  was  $14.57 \mu\text{g}/\text{m}^3$ . This finding suggested that the average concentration of  $PM_{0.1}$  was greater than 50% of the concentration of  $PM_{0.1-0.5}$ . When NPs are exposed for an extended period of time, it is probable that they will have a long-term effect on human health. The carbon composition revealed that the average concentration of OC was  $0.67 \mu\text{g}/\text{m}^3$ , while the average concentration of EC was  $0.36 \mu\text{g}/\text{m}^3$ , implying that OC was more concentrated than EC. This study site's source of NPs can be attributed to biomass burning.

*Keywords: Nanoparticle, Chemical Composition, Organic Carbon, Elemental Carbon*

# Interfacial Strengthening of Silicon Carbide Fiber via Electrophoretic Deposition of Modified Single-Walled Carbon Nanotube

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## Abstract

Fiber-reinforced composites (FRC) hold great promise for the aerospace and defense industries. Silicon carbide fiber, in comparison to carbon fiber, offers superior thermal resistance and possesses unique semi-conducting properties while retaining the mechanical characteristics of carbon fiber. However, its application in polymer matrix composites is restricted due to its inert surface. Researchers have conducted studies to modify the surface properties of the fiber to increase its adhesion to the polymer matrix, thereby enhancing its ability to transfer load stress from the resin to the fiber [1-3]. Nonetheless, many of the previously mentioned techniques are unsuitable for industrial mass production due to their complex processes and severe reaction conditions.[4] In this study, we draw inspiration from the widespread use of reinforced concrete structures in man-made buildings that surround us in daily life. By employing electrophoretic deposition (EPD) technique, carboxylated single-walled carbon nanotubes were deposited on various types of fiber. We created a moderately interconnected rigid structure on the fiber. This novel surface modification strategy is applied for simultaneous improvement of both interfacial shear strength (IFSS) and interlaminar shear strength (ILSS). The proposed method shows promise for producing low-cost, high-performance FRCs, and it offers an eco-friendly process in comparison to the former methods.

*Keywords: silicon carbide fiber, carbon fiber, electrophoretic deposition, carbon nanotube, surface modification.*

## Evaluation of AFM and TEM Dimensional Measurement Uncertainty of Nanoparticles Intercomparison Samples

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Mar Christian O. Que<sup>b</sup>, Alvin Kim M. Collera<sup>b</sup>

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### Abstract

This study presents the strategy used in the evaluation of the dimensional measurement uncertainty for nanoparticles used in the intercomparison organized by the Asia Nano Forum in 2019, with National Nanotechnology Center (NANOTEC) as the coordinating institute. Gold nanoparticles with size in the range from 20 nm to 100 nm were selected for the conducted interlaboratory comparison. The selected nanoparticles met the measurement requirements of Atomic Force Microscopy (AFM) and Transmission Electron Microscopy (TEM). The participating laboratories chose to conduct measurement using either methods or both. For the case of the Material Science Division (MSD) of the Industrial Technology Development Institute (ITDI), Department of Science and Technology (DOST) Philippines, both methods were used for the dimensional measurement. The comparison was performed as instrument based. In general, the instruments used were calibrated and capable of dimensional measurements in the nanometer-scale range to determine the sizes of the nanoparticles provided by the pilot laboratory. After analytical measurements were carried out, the uncertainty of measurement was carried using the bottom-up approach of ISO Guide 98-3 (ISO GUM). Uncertainty sources of significant contributions were identified and quantified, complying to the technical requirements of clause 7.6.1 of the international standard for the general requirements of the competence of testing and calibration laboratories, ISO/IEC 17025:2017. For AFM, the laboratory participated for the quantification of intercomparison samples coded G2, G5 and G6, and results obtained generated expanded uncertainties at 13% of the measured values, with coverage factor of 2 at 95% confidence interval. For TEM, the laboratory participated for the quantification of intercomparison samples coded G2, G3, G4, G5 and G6, and results obtained generated expanded uncertainties at 8% of the measured values, with coverage factor of 2 at 95% confidence interval.

*Keywords: Measurement uncertainty, AFM, TEM, nanoparticles, nanogold, interlaboratory comparison*

# Nanoscale Control in Heterogeneous Catalysis for a Sustainable Future

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## Abstract

Efficient utilization of transition metals is one of the most important requirements for heterogeneous catalysts. Design rules for nanoparticle catalysts are well established and often imply that sub-optimal metal dispersion is desired for high activity. Metal-support interactions can have a strong impact on the catalytic performance of metal nanoparticles. Specific sites at the metal-support interface can give rise to unusual high reactivity. In this contribution, I will review structure sensitivity for monometallic and bimetallic catalysts and demonstrate the possibility to tune metal-support interfaces towards high CO<sub>2</sub> hydrogenation and CO oxidation activity. The approach entails experimental work involving synthesis of uniform active phases, operando characterization, transient kinetic analysis augmented with density functional theory calculations of mechanism and microkinetics simulations. The first example deals with approaches to break structure sensitivity. For this, we use cobalt dispersed on ceria-zirconia support materials. We first establish how the size of the support crystallites can stabilize cobalt nanoparticles. Then, we investigate how incomplete reduction of cobalt oxide can lead to cobalt-cobalt oxide interfaces with a much higher CO<sub>2</sub> methanation activity than conventional cobalt nanoparticle catalysts. This work shows the promise of very small metal clusters stabilized on an oxide for achieving high CO<sub>2</sub> methanation activity.

Second, I will show how tuning the size of CeO<sub>2</sub> crystallites can strongly affect the stability and reactivity of single metal atoms. The improved reducibility displayed by CeO<sub>2</sub> particles of a few nanometer as contrasted to bulk CeO<sub>2</sub> with a size of tens of nanometers translates in retention of single Pd atoms with improved kinetics for low-temperature CO oxidation.

*Keywords: Catalysis, Structure sensitivity, Metal, Support, CO<sub>2</sub> hydrogenation*

## Short Bio:

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#### Professional Career

2009 – present Full Professor of Inorganic Materials and Catalysis & Head of laboratory; TU/e  
2022 – present Vice-dean of the Department of Chemical Engineering and Chemistry; TU/e  
2016 – 2020 Dean of the Department of Chemical Engineering and Chemistry; TU/e  
2016 Visiting Professor; Institute of Catalysis; Hokkaido University, Japan  
2008 – 2009 Associate Professor; Department of Chemical Engineering and Chemistry; TU/e  
2006 – 2008 Part-time researcher; Shell Research and Technology Center Amsterdam  
2002 – 2016 Part-time lecturer; Katholieke Universiteit Leuven  
2002 – 2007 Assistant Professor; Department of Chemical Engineering and Chemistry; TU/e  
2000 – 2001 Assistant Professor; Department of Technical Chemistry; University of Amsterdam

#### Education

1995 – 2000 PhD; Inorganic Chemistry and Catalysis, Eindhoven University of Technology  
1989 – 1994 Bachelor and Master; Chemical Engineering, Eindhoven University of Technology

#### Past and Present Professional Duties

- Chairman of the Netherlands Organization for Catalysis Research (NIOK)
- Member of the Board of Chemelot InSciTe (Institute for Science and Technology)
- Member of the Supervisory Board of the Institute for Sustainable Process Technology (ISPT)
- Principle investigator & management team member gravitation program “Multiscale Catalytic Energy Conversion (MCEC)”
- Member of the Advanced Research Center “Chemical Building Blocks Consortium”
- Member of the Board of the European Research Institute on Catalysis (ERIC)
- Member of the China Committee of the Royal Netherlands Academy of Arts and Sciences (2008-2016)
- Treasurer of the Dutch Zeolite Association (DZA)
- Member of ad-hoc committee formulating the Science and Technology Roadmap for Catalysis in the Netherlands: “Catalysis - Key to a Sustainable Future”
- Member of ad-hoc committee formulating the European Cluster on Catalysis Roadmap “Science and Technology Roadmap on Catalysis for Europe”
- Member of the Management Team of Catchbio SmartMix program (2011-2013); Program Leader “Lignin conversion” within the Catchbio SmartMix program (2013-2016)
- Member Program Council Chemical Conversion, Process Technology and Synthesis (Topsector Chemistry)
- Guest Editor of several special issues of scientific journals
- Member of International Scientific Advisory boards of several conferences (ICC, TOCAT, ABC)
- Member of editorial boards of Journal of Catalysis, Chinese Journal of Catalysis, Catalysis Communications, member of the advisory board of ACS Catalysis

# Formic Acid Synthesis from $\text{CO}_2 + \text{H}_2$ by Transition Metal-Chelated MOF-253: A Computational Chemistry Perspective

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## Abstract

The incorporation of transition metal elements within metal–organic frameworks (MOFs) is considered one of the most promising approaches for enhancing the catalytic capability of MOFs. MOF-253 ( $\text{Al}(\text{OH})(\text{dcbpy})$ ,  $\text{dcbpy} = 2,2'$ -bipyridine-5,5'-dicarboxylic acid), containing bipyridine coordination sites, has been theoretically investigated for potential transition metal chelation and subsequent  $\text{CO}_2$  reduction to formic acid. All transition metal elements from the third, fourth, and fifth periods, except hafnium and the lanthanide series, were considered in the characterization using density functional theory (DFT) calculations. Two distinct types of  $\text{CO}_2$  reduction mechanisms were identified for single-atom catalysts (SACs), namely: (1) the five-coordination Pd center promoting formic acid generation via an intramolecular proton transfer pathway; (2) several four-coordination metal centers (Mn, Pd, and Pt) generating formic acid through heterolytic hydrogen activation. The MOF-253 environment was found to introduce beneficial steric hindrance and constrain metal–ligand orientation to favor the formation of formic acid.

The formation of dual-atom catalysts (DUCs) was also explored based upon the various thermally-driven linker orientations. Explicit molecular dynamics simulations at different temperatures were conducted to analyze the interplay between guest molecule distribution and linker rotation. Ultimately, the favorable DUC sites were identified for converting  $\text{CO}_2 + \text{hydrogen}$  to formic acid through the collaborative metal redox processes, providing significantly more efficient pathway than the early SAC models. Powder X-Ray Diffraction (PXRD) patterns were simulated for the metal-chelated models to enable a comparison with the experimental observations in the literature.

**Keywords:** MOF-253,  $\text{CO}_2$  Reduction, Formic Acid Synthesis, Density Functional Theory, PXRD



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**Educational Background**

- 1997 B.Sc., Department of Applied Chemistry,  
National Chiao Tung University, TW  
2005 Doctor of Chemistry, College of Science, University of Pittsburgh, US (supervisor: Prof. Kenneth Jordan)

**Current Position**

- 2019- Full Professor, Chemistry Department, National Taiwan Normal University, TW  
2021- Adjunct Professor, Chemistry Department, Fu Jen Catholic University, TW  
2020- Director, Center for Cloud Computing, NTNU, TW

**Professional Experience**

- 2005-2007 Postdoctoral Researcher, Pacific Northwest National Laboratory, US  
2007-2009 Research Associate, Brookhaven National Laboratory, US  
2010-2015 Assistant professor, National Taiwan Normal University, TW  
2015-2019 Associate professor, National Taiwan Normal University, TW  
2017-2020 HPC Management Team Lead, Center for Cloud Computing, NTNU, TW

**Research Interests**

- 1) Computational Inorganic Chemistry in Renewable Energy Catalysis
- 2) Multiscale Modelling Method Development
- 3) Machine Learning for Materials and Molecule Design

**Awards**

Innovation-Oriented Trilateral Research Fund for Young Investigators of National Taiwan University System of 2017, 2019, 2020

**Recent Publications**

1. "Enhanced Predictions for the Experimental Photophysical Data Using the Featurized Schnet-base Approach", Sheng-Hsuan Hung, Zong-Rong Ye, Chi-Feng Cheng, Berlin Chen,\* Ming-Kang Tsai\*, J. Chem. Theory Comput. 2023, 19, 4559-4567 (cover highlight).
2. "Assessment of Predicting Frontier Orbital Energies for Small Organic Molecules Using Knowledge-Based and Structural Information", Zong-Rong Ye, Sheng-Hsuan Hung, Berlin Chen,\* Ming-Kang Tsai,\* ACS Engineering Au 2022, 2, 360-368 (cover highlight).
3. "Operando Time-resolved X-ray Absorption Spectroscopy to Unravel the Chemical Nature: Chemical State-Trapping Strategy Enabling the Highly Selective CO<sub>2</sub> Reduction", Sheng-Chih Lin, Chun-Chih Chang, Shih-Yun Chiu, Hsiao-Tien Pai, Tzu-Yu Liao, Chia-Shuo Hsu, Ming-Kang Tsai,\* Hao Ming Chen,\* Nat. Commun. 2020, 11, 3235.
4. "Predicting the Emission Wavelength of 10,000-plus Fluorescent Molecules by Clustering and Machine Learning Approaches", Zong-Rong Ye, I-Shou Huang, Yu-Te Chan, Zhong-Ji Li, Chen-Cheng Liao, Hao-Rong Tsai, Meng-Chi Hsieh, Chun-Chih Chang, Ming-Kang Tsai,\* RSC Adv. 2020, 10, 23834-23841.

# Nanostructured Electrodes as an Attractive Tool For Green Chemistry

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## Abstract

Over the last decades, the subject of complex interfaces has moved to the forefront of numerous original studies. The possibility to precisely engineer interfaces is playing an increasingly important role in the development of new technologies relevant to all aspects of our live, ranging from energy conversion to synthesis. Engineering of surfaces and interfaces simultaneously at different length scales, using self-ordering phenomena and growth processes can be steered to create a wide range of structures that allow the understanding of how structural features control the function of such systems.

Here we present electrochemical systems developed in the last few years using a rational design that allows us to fine-tune their physico-chemical properties by the controlled generation of metal nanostructures. Many electrochemical applications, including energy storage and conversion as well as electrocatalytic synthesis, require electrodes having a very large active surface, in order to achieve currents at a level sufficient for practical use. One way to reach this goal is to use porous materials.

In this presentation, we focus on the elaboration of original porous electrochemical interfaces with a very high degree of organization. We describe on the one hand macroporous electrodes obtained by hard molding [1], and on the other hand, mesoporous electrodes synthesized via a soft molding route [2]. We show recent examples illustrating these different elaboration strategies and the importance of such porous structures for the general purpose of green chemistry, especially for energy conversion [3-7] and the selective synthesis of high-added-value compounds [8-14].

*Keywords: Electrochemistry, Porous electrodes, Catalysis, Bioelectrochemistry*

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8. T Yuthalekha, C Wattanakit, V Lapeyre, S Nokbin, C Warakulwit, A Kuhn, **Nat. Comm.** 7 (2016) 12678
9. C Wattanakit, T Yuthalekha, S Assavapanumat, V Lapeyre, A Kuhn, **Nat. Comm.** 8 (2017) 2087
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11. S Butcha, S Assavapanumat, S Itisanronnachai, V Lapeyre, C Wattanakit, A Kuhn, **Nat. Comm.** 12 (2021) 1314
12. S Assavapanumat, S Butcha, S Itisanronnachai, A Kuhn, C Wattanakit, **Chemistry–An Asian Journal** 16 (2021) 3345-3353
13. S Butcha, V Lapeyre, C Wattanakit, A Kuhn, **Chem. Sci.** 13 (2022) 2339-2346
14. S Somsri, B Suwankaisorn, K Yomthong, W Srisuwan, S Klinyod, A Kuhn, C Wattanakit, **Chemistry–A European Journal** (2023) e202302054

**Short Bio: Prof. Dr. Alexander Kuhn**

Prof. Dr. Alexander Kuhn is Professor at the Institut of Molecular Science (University Bordeaux, CNRS, Bordeaux INP, France), as well as Adjunct Professor at VISTEC (Thailand) and Henan University (China). After studying chemistry at the TU München, he obtained his PhD in 1994 from the University Bordeaux. Following his post-doctoral studies at Caltech (1995/1996) he obtained an Assistant Professor (1996) and later a Full Professor (2000) position in Bordeaux. He is a senior member of the Institut Universitaire de France, distinguished senior member of the French Chemical Society, Fellow of the International Society of Electrochemistry and recipient of the CNRS Science Silver Medal. His current main research interests are modified electrodes with a special focus on applications in electroanalysis, bioelectrochemistry and electrocatalysis; nanomaterials; micro- and nanomotors; Janus particles; bipolar electrochemistry; chirality.

# Plasma Catalysis: Process Intensification at the Molecular Level

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## Abstract

Non-thermal plasma (NTP), low-temperature plasma or non-equilibrium plasma is the plasma which is not in thermodynamic equilibrium, is a promising, effective, and efficient technique to promote chemical reactions, especially in presence of a catalyst (known as the NTP catalysis), overcoming thermodynamic and/or kinetic barriers experienced by the conventional thermocatalysis. In NTP catalysis, the activation of reactant molecules could be primarily in gas discharge, being fundamentally different from that under thermal conditions and being able to enable process intensification at the molecular level. In addition, NTP catalysis is commonly operated under mild ambient conditions and able to couple the intermittent renewable energy (from solar farm and wind turbine) with short induction time, hence being suitable for developing the decentralized small-scale production technologies. NTP catalysis has been demonstrated suitable for activating the converting stable molecules such as CO<sub>2</sub> and N<sub>2</sub>, exemplified by CO<sub>2</sub> hydrogenation reactions and ammonia synthesis. However, to date, this emerging technology still suffers from the selectivity and efficiency issues, which requires further development. In this presentation, our research effort of exploring NTP catalysis, especially rational catalyst design for improving NTP catalytic processes, will be shared.

*Keywords: Non-thermal plasma (NTP), Catalysis, Process Intensification*

# Exploring a Novel Oxide State of Copper for Semiconductor Technology Materials

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## Abstract

The ability to create conductive copper coating layers and copper die-attach junctions through low-temperature sintering holds the promise of achieving enhanced functionality in high-performance semiconductors and power semiconductors at a more affordable cost. These semiconductors operate at exceptionally high temperatures, rendering traditional soldering techniques obsolete. Instead, a low-temperature sintering process is required. However, low-temperature sintering of copper presents a significant challenge. This is primarily due to the inherent ease with which copper nanoparticles oxidize, forming cuprous oxide and cupric oxide, making it impossible to simultaneously sinter at low temperatures.

To address this issue, we have synthesized novel nanoparticles by exerting control over their crystalline structure and surface oxidation state, enabling low-temperature copper atom diffusion. This breakthrough has paved the way for the creation of copper coatings with high conductivity and copper joints with significantly enhanced tensile strength, all achievable through low-temperature sintering.

This research breakthrough has opened up new avenues in the field of semiconductor technology. It offers the potential for producing high-performance semiconductor devices and power semiconductors with superior functionality at reduced production costs, while simultaneously addressing the challenges posed by high operating temperatures. This achievement signifies a vital step forward in advancing the capabilities of semiconductor technology and paves the way for more cost-effective and efficient solutions in the semiconductor industry.

The transition to innovative semiconductor technology in high-temperature environments where traditional soldering is challenging is expected to bring revolutionary advancements in energy efficiency and reliability. The use of copper through low-temperature sintering opens up new possibilities for the development of groundbreaking products, potentially revolutionizing the entire industry. The outcomes of this research position us to explore new horizons in future semiconductor technology.

*Keywords: Copper, nanoparticles, low temperature sintering, die-attach material, conductive material*

# Decoding Multimetallic Ensembles in Zeolite Pores: Towards Bias-Free Operando Modeling

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## Abstract

Zeolite and zeolite-based materials find a broad spectrum of applications as microporous catalysts in diverse chemical reactions. Their reactivity can be enhanced by introducing cationic complexes at extraframework positions, producing versatile catalytic ensembles.[1] These ensembles, when exposed to reaction conditions, can evolve, impacting their reactivity and catalytic behavior. Understanding their behavior under operation conditions is crucial for improved zeolite-based catalyst design.[2] In this lecture, I will present new computational strategies that integrate exhaustive configurational sampling, machine learning, and advanced ab initio thermodynamic analysis. This approach enables predictions of condition-dependent speciation and behavior of complex reactive ensembles in high silica zeolites. The methodological developments will be illustrated by our recent studies on the impact of extraframework aluminium species and synthesis conditions on the structure of metal-promoted Cu- [3] and Ga[4] oxo/hydroxo clusters in high-silica zeolites. The combination of unbiased ab initio configurational searches with advanced ab initio thermodynamic models opens up an exciting avenue to comprehend and direct the synthesis of multimetallic extraframework ensembles with optimal characteristics in confined space.

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[3] L. Tao, E. Khramenkova, I. Lee, T. Ikuno, R. Khare, A. Jentys, J.L. Fulton, A.A. Kolganov, E.A. Pidko\*, M. Sanchez-Sanchez, J.A. Lercher, *J. Am. Chem. Soc.* 2023, 145, 17710

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*Keywords: operando modeling; DFT calculations; zeolites; reaction mechanism; active site engineering*

**Short Bio: Prof. Dr. Evgeny Pidko**

Prof. Evgeny A. Pidko was trained physical chemistry at the Higher Chemical College of the Russian Academy of Sciences in Moscow, Russia and received Ph.D. in computational catalysis with prof. Rutger van Santen from Eindhoven University of Technology, the Netherlands (2005-2008), where in 2011-2017, he was an Assistant Professor of Catalysis for Sustainability. He spent summer 2012 as a visiting professor in the group of Prof. Christophe Coperet at ETH Zurich to learn the art and science of synthetic organometallic chemistry. In 2016 he obtained an ERC Consolidator grant “DeLiCat” to learn, understand and control the deactivation phenomena in hydrogenation catalysis. In September 2017, he moved to Delft University of Technology to become an Associate Professor and head of the Inorganic Systems Engineering group at the Chemical Engineering Department, where he was promoted to Full Professor in 2020. In summer 2023, he served a visiting professor at the Institute for Catalysis at Hokkaido University. He is a member of the advisory boards of ChemCatChem and Catal. Sci. Technol. journals, and an editorial board member of Kin. Catal. and Mend. Commun. journals. He is an author of >230 publications on various topics of computational, physical, inorganic, supramolecular chemistry, catalysis, and chemical engineering. His research aims at understanding and development of catalytic systems for sustainable chemical processes including experimental and computational studies of the mechanisms and property-activity relationships in organometallic and molecular heterogeneous catalysis. Besides science, Evgeny enjoys diverse literature and music, cooking and spending quality time with his wife Svetlana and their kids Sasha and Stepan.



# Theoretical Understanding on Carbon-Carbon Coupling Reaction on B-doped Graphyne from Bond Order Conservation

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## Abstract

Due to the issue of global warming, efficient utilization of CO<sub>2</sub> has been an important topic. Electrocatalytic reduction of CO<sub>2</sub> to C<sub>2+</sub> products such as C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>5</sub>OH, or C<sub>3</sub>H<sub>7</sub>OH is an ideal solution. However, applications have been hindered by the slow kinetics due to the very high barrier of the Carbon-Carbon coupling (CC coupling) reaction. In this study, we focus on non-metal doping to 2D-carbon materials and theoretically evaluate the potential of boron doping to the sp linker of the sp-sp<sup>2</sup> hybrid graphyne. We rationalized our finding by evaluating the bond order as well as the ground and excited electronic states of the adsorbates.

In many previous studies, hetero-atom doping has focused on sp<sup>3</sup> and sp<sub>2</sub> hybrid materials such as nanodiamond or graphene. However, we could not find any examples of efficient CC coupling reactions on these systems. Here we looked at the reaction on boron doped graphyne, which is a new allotrope of carbon containing both sp<sup>2</sup> (benzene knots) and sp (acetylene linkers) hybridization. On this interesting surface, we found the CC coupling barrier to be very low at 0.4 eV. Analyzing the bond order index along the reaction path, we found that the acetylene linkers change from triple to single to double bond hybridization as the reaction proceeds from \*+2CO→2\*CO→\*OCCO. This flexible change of the acetylene linker allows for bond order conservation as the CC coupling reaction proceeds. We also found that bond order conservation can be rationalized by looking at the orbital occupation flipping of the HOMO and LUMO as the CC coupling reaction proceeds. We believe such a new mechanism for CC coupling will open up new ideas for the efficient production of C<sub>2+</sub> products.

*Keywords: bond order conservation, quantum chemistry, orbital crossing, crystal orbital bond index*



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**PROFESSIONAL EXPERIENCE**

Associate Research Fellow, 2017 January  
Institute of Atomic and Molecular Sciences, Academia Sinica Taipei, Taiwan (R.O.C.)  
Assistant Research Fellow, 2009 June-2017,  
January Institute of Atomic and Molecular Sciences, Academia Sinica Taipei, Taiwan (R.O.C.)  
Postdoctoral Fellow, 2006 October-2009 April  
Department of Chemistry and Biochemistry, University of Colorado at Boulder, Boulder, Colorado, U. S. A.  
Postdoctoral Fellow, 2005 April-2006 September  
Institute of Atomic and Molecular Sciences, Academia Sinica Taipei, Taiwan (R. O. C.) Research  
Assistant, 2003 April-2005 March Keio University, Yokoyama, Japan

**ACADEMIC BACKGROUND**

Ph.D. in Science, Graduate School of Science and Technology, Keio University, Yokohama, 2005  
Advisor: Dr. Satoshi Yabushita  
M.S., Graduate School of Science and Technology, Keio University, Yokohama, 2002  
Advisor: Dr. Satoshi Yabushita

**CURRENT RESEARCH INTERESTS**

Theoretical calculation of vibrational spectra  
Rate calculation with anharmonic corrections  
Modelling of reactions on metal surface  
Photoinduced reactions  
Electronic structure calculation for couple electronic states

**RESEARCH SKILLS**

Quantum chemistry calculation using the ACES II, COLUMBUS, GAMESS, Gaussian, and MOLPRO programs  
Quantum dynamics calculation using ABC and MCTDH programs  
Programming using FORTRAN and Mathematica  
Fond with using Linux, Unix, Windows, and Macintosh machines

# Simulations on Ion-Dynamics-Related Properties of Nanomaterials via Machine Learning Potentials

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## Abstract

Understanding on ion-dynamics-related properties such as ionic conductivity, thermal conductivity and catalytic activities of nanomaterials is of importance in developing nanomaterials that can contribute much to solve global energy issues. First-principles calculations are powerful in deepening such understanding because of their excellent prediction ability. However, their high computational cost sometimes makes realistic modeling of target systems difficult. In this context, machine learning potentials (MLPs) have attracted much attention recently because they are expected to achieve prediction accuracy comparable to first-principles calculations and feasible computational costs simultaneously. In this presentation, we will introduce our recent simulations on ion-dynamics-related properties of nanomaterials using MLPs, together with development of new schemes for enabling investigation of situation/factor which cannot be taken into account by the conventional MLPs.

Specifically, we will talk on the following topics. 1) Ion transport properties of  $\text{Li}_3\text{PO}_4$  [1,2]: Besides demonstrating accurate prediction on Li diffusion behavior [1], a new MLP scheme that can consider the effects of applied electric fields and interesting Li behavior in amorphous  $\text{Li}_3\text{PO}_4$  under an electric field found in our simulation are described [2]. 2) Thermal properties of nitride semiconductors [3]: A new MLP scheme to take account of multiple charge states of defects [3] is described, and the effects of charge state on phonon dispersion and thermal conductivity are discussed. 3) Catalytic activities of high entropy alloy nanoclusters: Toward exploration of high entropy alloy nanoclusters that simultaneously satisfy both high stability and catalytic activity, we have been constructing MLPs in a way that uses a relatively small number of data. Preliminary results on this topic will be presented.

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*Keywords: Machine learning potential, ion transport, thermal transport, catalysis*

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<The organizers of NanoThailand may use one of the following as they like. If adjustment of length is necessary, please feel free to contact me.>

**CV #1**

Satoshi Watanabe received his Ph.D. degree in Physics from The University of Tokyo in 1989. He worked on the Aono Atomcraft Project at the Research Development Corporation of Japan from 1989 to 1994 and at the Advanced Research Laboratory, Hitachi Ltd. from 1994 to 1997. Afterwards, he joined The University of Tokyo in 1997 as an associate professor of Department of Materials Engineering and became a professor in 2004. He has also been a special advisor to the president, The University of Tokyo, since 2019. His research fields are computational materials physics, electronic structure calculations, nanoscale transport, nanomaterial properties, and materials informatics.

**CV #2**

**EDUCATION** 1984 B. Sci.: Department of Physics, School of Science, The University of Tokyo  
1986 M. Sci.: Department of Physics, School of Science, The University of Tokyo  
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**WORKING EXPERIENCE**

1989-1994 Researcher, Aono Atomcraft Project, Research Development Corporation  
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1994-1997 Visiting Researcher, Advanced Research Laboratory, Hitachi, Ltd.  
1997-present Department of Materials Engineering, The University of Tokyo  
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2019-present Special Advisor to the President, The University of Tokyo

**RECENT PROJECT**

- 1) Theoretical analyses on ionic transport in resistive switches, all solid-state batteries, and related systems
- 2) Theoretical analyses on phonon-related properties in solids
- 3) Construction and application of machine-learning interatomic potentials to the above problems

**HONORS AND AWARDS**

2011 Fellow, Surface Science Society of Japan  
2021 JVSS Award, The Japan Society of Vacuum and Surface Science

# Utilization of CO<sub>2</sub> Using Nanostructured Heterogeneous Catalysts

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## Abstract

The catalytic activity and selectivity of heterogeneous catalysts are very much dependent on their morphology and structure. In spite of the great technological, environmental, and economic interests, general methods for the activation and utilization of CO<sub>2</sub> are missing to be developed. The talk will cover our recent progress in the synthesis of nanostructured materials, their characterization, and their application. The materials have been applied as heterogeneous catalysts for the utilization of CO<sub>2</sub> into fuels and chemicals. Several different catalytic systems were developed where various types of metal nanoparticles are incorporated into different types of porous and nanostructured materials. The methods aim to be cost-effective and practical and result in a narrow size distribution of small uniform nanoparticles. More importantly, the catalysts show high activity and selectivity in various reactions. We present the progress that has been made in the synthesis in various ways and their characterization using different techniques. We have especially focused on novel materials with high catalytic selectivity for hydrogenation of CO<sub>2</sub> into CO, CH<sub>4</sub>, methanol, and ethanol respectively.

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- [6] F. Goodarzi, M. K. Larsen, J. Mielby, S. Kegnæs, *J. CO<sub>2</sub> utilization*, 2023

**Keywords:** Catalysis, CO<sub>2</sub>, C1 chemistry, nanoparticles, porous materials

**Short Bio: Søren Kegnæs**

**PERSONAL INFORMATION**

Name: Søren Kegnæs, (Søren Kegnæs Klitgaard until 2009)  
Date of birth: March 12, 1980, Denmark. Nationality: Danish-Swedish  
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**EDUCATION**

2012 HD 1, Graduate Certificate in Business Administration, Copenhagen Business School, Denmark.  
2009 Ph.D. degree (Chemistry, 1/4-2009), Technical University of Denmark, Denmark.  
2005 Master degree (M.Sc. in Chemistry, 1/11-2005), University of Copenhagen, Denmark.  
2003 Bachelor degree in Chemistry-Other (Computer Science), University of Copenhagen, Denmark.

**WORK EXPERIENCE**

2022 – Professor (Faculty), DTU Chemistry, Technical University of Denmark, Denmark.  
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2017 – 2022 Professor (MSO; Faculty), DTU Chemistry, Technical University of Denmark, Denmark.  
2014 – 2017 Associate Professor (Faculty), DTU Chemistry, Technical University of Denmark, Denmark.  
2009 – 2013 Assistant Professor(Faculty)/Post Doc,  
DTU Chemistry, Technical University of Denmark, Denmark.  
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2011 Post Doc research project funded by Eastman Chemical Company, Texas, USA.  
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2005 – 2009 PhD student, Department of Chemistry, Technical University of Denmark, Denmark.  
2002 – 2005 Teaching assistant, Department of Chemistry, University of Copenhagen.  
2015 Paternity leave (0.5 month, 03-16/05/2015)  
2012 Paternity leave (0.5 month, 13-26/06/2012)

**AWARDS AND HONORS**

2023 The Novo Nordisk Foundation Distinguished Innovator.  
2016 The Danish Council for Independent Research (DFF) - Sapere Aude: Starting Grant  
2016 VILLUM FONDEN Young Investigator  
2015 “Betty og Valdemar van Hauens Fond” - Honorary award.  
2011 Danish Ministry of Science, Technology and Innovation’s Young Elite Researcher

**EXTERNAL FUNDING FOR RESEARCH PROJECT**

2010 – 2022 > 5.0 M € in grants and external funding for research projects as Principal Investigator. In total ~10.5 M € including research grants and funding as co-Principal Investigator.

# Metal-Organic Frameworks (MOFs)-Driven Carbon Neutral Society: Heterogeneous Catalysis of Waste Biomass and Plastics Conversion

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## Abstract

Scientific innovation in various fields is surely necessary to achieve carbon neutrality by 2050. To reduce carbon dioxide (CO<sub>2</sub>), seven approaches including de-fossil resources, switch to renewable energy, etc. have been proposed. Meanwhile, nanoporous metal-organic frameworks (MOFs) have been well known and have shown great potential in catalysis and energy applications owing to their high surface areas, controllable composition, and tunable surface functionalities. In this talk, I will focus on MOFs-driven carbon neutral society by introducing MOFs in waste biomass and plastics conversion. (1) For heterogeneous catalysis, we synthesize a heterogeneous Bi-BTC catalyst for the conversion of bio-based 2,5-dimethylfuran and acrylic acid to para-xylene with a promising yield (92%), under relatively mild conditions (160 °C, 10 bar) with low reaction energy barrier (47.3 kJ/mol). The proposed reaction strategy also demonstrated remarkable versatility for furan derivatives such as furan and 2-methylfuran. (2) For plastics conversion, polyethylene terephthalate (PET) has been extensively used for fabrication of various packaging materials, creating million tons of waste per year. Degrading and recycling PET waste has been identified as a prominent issue. Herein, we demonstrate an effective process to chemically convert PET to bis(2-hydroxyethylterephthalate) (BHET) through the use of metal azolate framework-6 (MAF-6) as a catalyst in the presence of ethylene glycol. A high 92.4% conversion of PET and 81.7% yield of BHET at 180 °C for 4 h was achieved. We have also hypothesized a mechanism for the high conversion and yield of PET glycolysis reaction catalyzed by MAF-6.

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- Highly Selective and High-Performance Osmotic Power Generators in Subnanochannel Membranes Enabled by Metal-Organic Frameworks. *Science Advances*. 2021, 7, eabe9924.
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- Yu-Wen Chiao, Weisheng Liao, Philip Anggo Krisbiantoro, Bor-Yih Yu\*, Kevin C.-W. Wu.\* Waste-Battery-Derived Multifunctional Zinc Catalysts for Glycolysis and Decolorization of Polyethylene Terephthalate. *Applied Catalysis B: Environmental*. 2023, 325, 122302

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2001-2005 Ph.D., Dept. of Mater. Sci. Eng., The University of Tokyo, Tokyo, Japan  
1994-2000 B.S. & M.S., Dept. of Agri. Chem., National Taiwan University, Taipei, Taiwan

**3. Current position and relevant experience**

2016-present Professor, Dept. of Chem. Eng., National Taiwan University  
2019-present Director, Division of Strategic Planning, Office of Research and Development, National Taiwan University  
2018-present Professor, Molecular Science & Technology, National Taiwan Univ. (NTU-MST)  
2010-present Joint Appointed Investigator, National Health Research Institutes, Taiwan  
2014-2016 Secretary General, Taiwan Institute of Chemical Engineers  
2012-2016 Associate Professor, Dept. of Chem. Eng., National Taiwan University  
2013-2016 Vice chair, The Center of Strategic Materials Alliance for Research and Technology (SMART Center), National Taiwan University, Taipei, Taiwan  
2008-2012 Assistant Professor, Dept. of Chem. Eng., National Taiwan University  
2006-2008 Post-doc, Dept. of Chem., Iowa State Univ., Iowa, USA  
2005-2006 Post-doc, Dept. of Applied Chem., Waseda Univ., Tokyo, Japan

**4. Major awards and honours (Recent five years)**

2018: Humboldt scholars, Research Fellowship for Experienced Researchers from Alexander von Humboldt Foundation, Germany, 2018-2020.

2018: Outstanding Research Award, Ministry of Science and Technology, Taiwan.

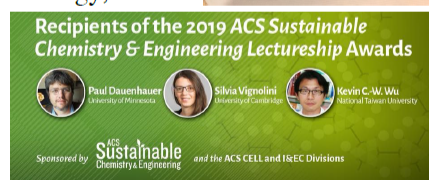
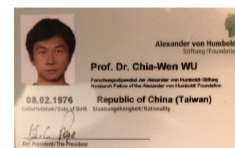
2019: ACS Sustainable Chemistry & Engineering Lectureship Award (ACS)

2019: Outstanding Researcher Award (Asia-Pacific Association of Catalysis Societies; APACS)

2019: Outstanding Young Scholar Award, LCY Education Foundation.

2020: Outstanding Research Award, Ministry of Science and Technology, Taiwan.

2021: Clarivate Highly Cited Researchers (Cross-fields)



# Towards Ultrahigh Osmotic Power Harvesting by Metal-Organic Frameworks and Covalent-Organic Frameworks

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## Abstract

The chemical energy stored between seawater and river water, the so-called osmotic power (or blue energy), can be harvested by an ion-selective membrane. However, previously reported membranes suffer from insufficient ion selectivity and inferior transmembrane ionic flux (low conductance), thus impeding practical application. For example, the output osmotic power density reported by most of existing ion selective membranes is typically below the commercial benchmark of 5 W/m<sup>2</sup>. Taking the inspiration from electrocytes in electric eel, which consist of a large number of sub-nanoscale rectified ion channels that allow unidirectional ion transport with amplified flux, we engineered two types of sub-2 nm-scale metal-organic framework (MOF) and covalent-organic framework (COF)-based ionic diode membranes for osmotic power harvesting. We show that the two MOF and COF-based heterogeneous membranes can rectify ionic current even in high salt concentration. We then probe application of these membranes in harvesting energy from salinity gradients. Notably, in addition to ultrahigh ion selectivity, these sub-2 nm-scale ionic diode membranes can achieve an unprecedented power density, higher than the commercial benchmark bandgap and outperforms all the state-of-the-art ion selective membranes. Our works would open up new avenues of using pinhole-free MOF and COF membranes towards next-generation highly selective and ultrahigh-performance sustainable energy harvesting.

*Keywords: Blue energy, Ion transport, Ionic diode, Metal-organic framework, Covalent-organic framework*



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**Education**

Ph.D. in Chemical Engineering, National Taiwan University, Taiwan (2017)

**Research Interests**

Microfluidics and Nanofluidics  
Ion Transport Membrane  
Water-Enabled Energy  
Metal-Organic Framework/Covalent-Organic Framework  
Colloid and Interface Science

**Honors**

1. Outstanding Research Award, National Science and Technology Council, Taiwan, 2023.
2. The SCEJ Award for Outstanding Asian Researcher and Engineer, The Society of Chemical Engineers (SCEJ), Japan, 2020.
3. Ta-You Wu Memorial Award, Ministry of Science and Technology, Taiwan, 2019.

**Representative Publications**

1. C. W. Chu, A. R. Fauziah, L. H. Yeh,\* “Optimizing Membranes for Osmotic Power Generation”, *Angewandte Chemie International Edition*, 62, e202303582 (2023).
2. K. T. Huang, W. H. Hung, Y. C. Su, F. C. Tang, L. D. Linh, C. J. Huang,\* L. H. Yeh,\* “Zwitterionic Gradient Double-Network Hydrogel Membranes with Superior Biofouling Resistance for Sustainable Osmotic Energy Harvesting”, *Advanced Functional Materials*, 33, 2211316 (2023).
3. M. Gao, M. J. Zheng, A. F. M. EL-Mahdy, C. W. Chang, Y. C. Su, W. H. Hung, S. W. Kuo,\* L. H. Yeh,\* “A Bioinspired Ionic Diode Membrane Based on Sub-2 nm Covalent Organic Framework Channels for Ultrahigh Osmotic Energy Generation”, *Nano Energy*, 105, 108007 (2023).
4. Y. C. Liu, L. H. Yeh,\* M. J. Zheng, K. C. W. Wu,\* “Highly Selective and High-Performance Osmotic Power Generators in Subnanochannel Membranes Enabled by Metal-Organic Frameworks”, *Science Advances*, 7, eabe9924 (2021).
5. J. P. Hsu, T. C. Su, P. H. Peng, S. C. Hsu, L. H. Yeh,\* “Unraveling the Anomalous Surface-Charge-Dependent Osmotic Power Using a Single Funnel-Shaped Nanochannel”, *ACS Nano*, 13, 13374-13381 (2019).
6. C. Y. Lin, C. Combs, Y. S. Su, L. H. Yeh,\* Z. S. Siwy,\* “Rectification of Concentration Polarization in Mesopores Leads To High Conductance Ionic Diodes and High Performance Osmotic Power”, *Journal of the American Chemical Society*, 141, 3691-3698 (2019).



# Green Energy and Water Cleanup: Biocrude Production and Advanced Remediation of Carbon and Nitrogen-Enriched Wastewater

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## Abstract

Biomass is a sustainable carbon resource with vast potential for producing various liquid fuels and chemicals. When subjected to hydrothermal conditions, biomass components undergo degradation, resulting in various oxygenates that find applications in current and future industrial sectors. Hydrothermal conditions offer distinct advantages compared to other thermochemical conversion processes. These benefits include wet feedstocks, enhanced separation of reaction products, and significantly reduced reaction times for biomass depolymerisation, transforming hours into minutes when contrasted with conventional acid hydrolysis at atmospheric pressure.

This presentation focuses on the fundamental aspects of biomass component decomposition under hydrothermal conditions. It follows a two-fold approach: first, experimental characterisation of biomass liquefaction in well-suited reactor systems; second, a scoping study of an electro-oxidation process for treating wastewater streams containing representative organic pollutants downstream. Emphasis will be placed on establishing a framework for selecting and optimising experimental techniques suitable for a range of biomass feedstocks and wastewater treatment processes within the biochemical manufacturing industry.

# Macroscopic Shaping of Monolithic Catalyst via Crystal-Glass Transformation of Coordination Polymer

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## Abstract

Coordination polymers (CPs) and the related metal-organic frameworks (MOFs) are coordination compounds of metal ions and bridging ligands with extended structure. Recently, CP/MOF glasses with preserved short-range order have emerged as a new class of materials. They exhibit the distinct properties from their crystalline counterparts, for example, optical transparency, mechanical stability, soft nature, and ionic/electronic conductivities. CP/MOF glasses can be obtained via the crystal-glass phase transformation induced by melt-quenching and mechanical milling. Motivated by the moldable character of melting CP/MOFs, we performed the macroscopic shaping of CP/MOF catalyst without using the secondary components to circumvent the difficult processibility and recovery of catalyst powder. For example,  $[\text{Zn}_3(\text{H}_2\text{PO}_4)_6(\text{H}_2\text{O})_3](\text{HbIm})$  (ZnPbIm; HbIm: 1,3-benzimidazole) consisting of zinc ions, orthophosphates, and benzimidazoles was chosen as an example to realize the shape engineering of monolithic catalysts into different shapes and sizes. Given the macroscopic form, facile catalyst recovery was achieved with over 90% of catalyst mass recovered in the liquid-phase levulinic acid esterification. In addition, the dense structure of glass is expected to prevent the migration of catalytic nanoparticles during the catalysis. The recrystallization of glass could be helpful for the confinement of metal nanoparticles during the rearrangement of metal ions and organic ligands. The perspectives of utilizing the phase transformation of CP/MOFs for the preparation of self-supporting monolithic catalyst and the metal nanoparticle confinement will also be discussed.

**Keywords:** Coordination polymer (CP), metal-organic framework (MOF), phase transformation, heterogeneous catalysis, catalyst

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2018 – 2020 Postdoctoral Fellow, School of Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology (VISTEC), Thailand

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2013 – 2018 Ph.D. in Chemical Engineering, Kasetsart University, Thailand  
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2013 – 2018 The Royal Golden Jubilee Ph.D. Scholarship, the Thailand Research Fund (TRF) and Kasetsart University  
2015 – 2016 Visiting Ph.D. Student at Vienna University of Technology (TU Wien), Austria

# Photo-Induced Electrochemiluminescence at Nanostructured Semiconductor Surfaces

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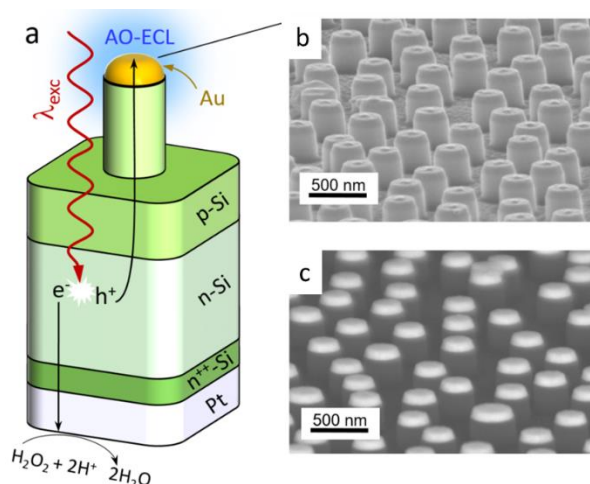
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## Abstract

Photoelectrochemistry at semiconductor electrodes combines photon absorption and electrochemical charge transfer. The simultaneous occurrence of both processes allows for triggering electrochemical reactions with a considerably lowered energy input. So far, this phenomenon has been proven very promising for solar-to-fuel conversion applications.<sup>1</sup> On the other hand, electrochemiluminescence (ECL) is a light-emitting process and a powerful technique in analytical chemistry, successfully commercialized for immunoassays.<sup>2</sup> This phenomenon is induced by the excited state of a luminophore, which is generated by an electrochemical reaction at an electrode surface. We have explored the combination of photoelectrochemistry and ECL, referred to as photoinduced ECL (PECL),<sup>3</sup> to generate original Stokes<sup>4</sup> and anti-Stokes<sup>5</sup> light conversion schemes. More recently, we designed an all-optical monolithic photoelectrochemical device that generates ECL photons autonomously under a remote light stimulus, without the need for any electrical power supply, wires, electrodes, connections, and specific electrochemical knowledge.<sup>6</sup> The approach is based on a nanostructured Si photovoltaic junction modified with catalytic coatings to generate ECL under illumination with a light-emitting diode. It constitutes the first electrically-autonomous and the simplest ECL configuration reported to date.<sup>6</sup> This breakthrough provides a general strategy for generalizing ECL. Given the crucial importance of ECL technologies for medical diagnosis, this concept opens important opportunities for the development of wireless point-of-care sensing devices and imaging strategies with considerable ease-of-use.



**Keywords:** Electrochemiluminescence, photoelectrochemistry, light upconversion, nanostructured Si photovoltaic junction

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6. Zhao, Y.; Descamps, J.; al Hoda Al Bast, N.; Duque, M.; Esteve, J.; Sepulveda, B.; Loget, G.; Sojic, N. *J. Am. Chem. Soc.* **2023**, DOI: 10.1021/jacs.3c05856.

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**Education/Experiences:**

- 1997 PhD - Ecole Normale Supérieure – Université Pierre et Marie Curie/ Paris VI
- 1998 Post-doc – Department of Chemistry, University of Texas at Dallas
- 2004 Habilitation at the University of Bordeaux

**HONORS:**

- 1998 Robert A. Welch Foundation Fellow.
- 2005 French Chemical Society - Analytical Chemistry Division Medal.
- 2010 Guest Professor Max Planck Institute of Colloids and Interfaces, Potsdam, Germany
- 2011 Distinguished Lecturer at the University of Belgrade, Serbia
- 2015 Guest Professor University of Bologna, Italy
- 2022 Invited visiting Professor University of Venice, Italy
- 2022 Chinese Academy of Science President's International Fellowship

**Other Activities**

Associate editor of the journal “*Chemical & Biomedical Imaging*” published by the American Chemical Society (<https://pubs.acs.org/journal/cbihbp>)

**Publications**

Author of more than 200 peer reviewed papers, 11 book chapters, 1 book and 7 patents, which have attracted over 5000 citations. H-Index: 46.

# Bulk Electroenzymatic Synthesis with Microelectrodes by Bipolar Electrochemistry

Lin Zhang,<sup>a,\*</sup> Chunhua Zhang,<sup>a</sup> Alexander Kuhn<sup>a,b</sup>

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## Abstract

Electrochemical regeneration of reduced nicotinamide adenine dinucleotide (NADH) is an extremely important challenge for the electroenzymatic synthesis of many valuable chemicals. Although important progress has been made with modified electrodes with respect to the reduction of NAD<sup>+</sup>, the scale-up is difficult due to mass transport limitations inherent to large-size electrodes. Here, we propose to employ a dispersion of modified electrocatalytically active microparticles in the bulk of a bipolar electrochemical cell. In this way, redox reactions occur simultaneously on all of these individual microelectrodes without the need of a direct electrical connection. The concept is first validated by using [Rh(Cp\*)(bpy)Cl]<sup>+</sup> functionalized carbon microbeads, acting as bipolar objects, for the electroregeneration of enzymatically active 1,4-NADH at the negatively polarized face of the particles (Scheme 1). The efficiency of the system can be fine-tuned by controlling the electric field in the reaction compartment and the number of dispersed microelectrodes [1].

Furthermore, we propose to use such type of functionalized glassy carbon beads suspended in a bipolar electrochemical cell for bulk electroenzymatic synthesis. The beads are in this case modified with a metal–organic framework NU-1000 shell, in which [Rh(Cp\*)(bpy)Cl]<sup>+</sup> catalyst is incorporated via the solvent-assisted ligand incorporation approach [2]. Enzymatically active 1,4-NADH is electrochemically regenerated, allowing the efficient bipolar electrochemical bulk conversion of pyruvate into L-lactate in the presence of NADH dependent L-lactate dehydrogenase as a model system. The very high turnover frequency (TOF) of 3100 ± 106 h<sup>-1</sup> opens up promising perspectives for employing this concept also for various other electroenzymatic bulk processes [3].

**Keywords:** Bipolar electrochemistry, Electroenzymatic synthesis, NADH regeneration

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- [2] W. Li, C. Zhang, Z. Zheng, X. Zhang, L. Zhang, A. Kuhn, *ACS Appl. Mater. Interfaces* 2022, 14, 46673–46681
- [3] C. Zhang, X. Zhang, Y. Fu, L. Zhang, A. Kuhn, *J. Catal.* 2023, 421, 95–100.

**Short Bio: Professor Lin Zhang**

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**EXPERIENCE**

2020.06-Present:	Professor, Henan University, China
2019.01-2020.06:	Special-term Professor, Henan University, China
2017.02-2018.10:	Postdoctoral researcher, University of Bordeaux, France under the supervision of Prof. Alexander Kuhn

**EDUCATION**

2013.11-2016.12:	Ph.D. in Physical Chemistry, University of Lorraine, Nancy, France under the supervision of Dr. Mathieu Etienne
2011.10-2013.06:	Master in Physical Chemistry, University of Bordeaux, France; Master in Advanced functional Materials, University of Augsburg, Germany
2003-2006:	B.Sc. in Chemistry, Faculty of Chemistry, China

**RESEARCH FIELD**

Construction of functional electrodes for cofactor NADH regeneration  
Bipolar electrochemistry and its application in electrocatalytic synthesis



# Electromechanical Systems for the Enantioselective Wireless Loading and Release of Fluids

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## Abstract

Chirality plays an important role in multiple fields of science such as chemistry, biology or medicine. Although enantioselective separation of chiral molecules, induced by external stimuli, has been well established, [1] the development of miniaturized chiral soft systems able to quickly and wirelessly distinguish such molecules still faces great challenges. The synergy between the mechanical properties and the enantioselectivity of conjugated polymers powered by bipolar electrochemistry (BE) could lead to so far unexplored effects. Through this approach, we have prepared soft tubes [2] and actuators [3] that mimic either chiral columns or chiral valves commonly used in the field of chiral chromatography and microfluidic, respectively. Furthermore, the wireless mode, an intrinsic feature of BE, is an added value that allows to achieve the recognition and/or separation of chiral molecules in a cheap and fast way.

[1] Salinas G., Arnaboldi S., Bouffier L., Kuhn A. *ChemElectroChem* **2022**, 9, e202101571.

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[3] Salinas G., Malacarne F., Bonetti G., Cirilli R., Benincori T., Arnaboldi, S., Kuhn A. *Chirality* **2023**, 35, 110.

*Keywords: chirality, chiral separation, wireless mode, electric field, miniaturized devices*

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**Short Bio: Assoc. Prof. Serena Arnaboldi**

Serena Arnaboldi is an Associate Professor in Analytical Chemistry at Department of Chemistry, University of Milan (Italy). She achieved a PhD in 2014 under the supervision of Patrizia Mussini at the University of Milan. After a period spent as post-doctoral fellow in the same group in Milan, she moved to Bordeaux in Alexander Kuhn' s group. In 2021 she was awarded with an ERC Starting Grant for a project concerning the transmission of chirality across length scales. Her main research interest is chiral electrochemistry, including; enantioselective electroanalysis, enantioselective electrosynthesis, (chiral) bipolar electrochemistry, (chiral) ionic liquids and self-propelled electrochemical actuators.

# Magnetic Field-Enhanced Self-Electrophoretic Propulsion for Enantioselective Synthesis with Nanostructured Microswimmers

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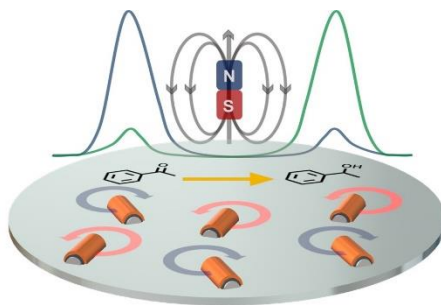
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## Abstract

Over the last 40 years, the so-called magnetohydrodynamic effect has been an interesting alternative to enhance mass transport in different electrochemical systems. The spatial distribution of the magnetic field, with respect to the working electrode, induces a Lorentz force on the ionic flux, leading to a controllable hydrodynamic convection.<sup>(1,2)</sup> Recently, this concept was applied to self-electrophoretic swimmers in order to boost their kinetic energy.<sup>(3)</sup> The presence of the magnetic field induces the formation of circular vortexes in the electrolyte at each extremity of the device and a torque force, producing a controllable clockwise or anticlockwise trajectory. Furthermore, the Lorentz force, which is responsible for creating the hydrodynamic convection in these self-induced polarized systems, allows for bypassing mass transport limitations in novel and unconventional processes.

In this work, we take advantage of the synergy between the magnetic field-enhanced self-electrophoretic propulsion mechanism and the enantioselective redox chemistry on-the-fly in order to boost stereoselective conversion.<sup>(4)</sup> In the presence of an external magnetic field, the designed Janus redox micro-reactors exhibit well-controlled clockwise or anticlockwise motion with an enhanced speed. By using the thermodynamically spontaneous oxidation of Zn, as a source of electrons together with the outstanding enantioselectivity of an inherently chiral oligomer, these hybrid objects convert spontaneously on-the-fly a prochiral molecule into a specific enantiomer with high enantiomeric excess. Finally, the magnetic field-enhanced self-mixing induced by the swimmers, based on the formation of local magnetohydrodynamic vortices, leads to a significant improvement in reaction yield and conversion rate.



**Keywords:** Lorentz Force, Magnetohydrodynamics, Chemistry on-the-fly, Enantioselective synthesis.

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## Accelerating Circular Economy Initiatives for a Sustainable Future

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### Abstract

The pursuit of a sustainable future has fostered the convergence of biomass innovation and circular economy principles, facilitating resource efficiency and waste reduction. Biomass innovation within the circular economy framework focuses on harnessing organic waste streams for valuable products and applications. The conversion of empty fruit bunches (EFB) and oil palm waste, to nanocellulose and graphene represents a compelling advancement in this field. Nanocellulose, derived from the fibrous EFB material, possesses good mechanical strength by adding nanocellulose as a reinforcement in polymer composites, which is valuable for automotive coatings and construction materials. Furthermore, nanocellulose being organic can support cell growth and tissue formation, making it suitable for wound care application and finally nanocellulose are also used as additives in drilling fluids in the oil and gas industry as its high aspect ratio provides reinforcement and stability. Through innovative processes, graphene can also be synthesized from the oil palm waste such as palm trunk, palm kernel shell and biomethane from the palm oil mill effluent (POME), offering a high surface area property where it can be employed as additives to rubber, plastics and composites, acts an efficient oil and heavy metal adsorbent in water purification processes, and high energy density, fast charging battery applications. For example, the addition of graphene enhances the rubber's mechanical properties, such as tensile strength, hardness, and wear resistance. Additionally, this paper highlights the potential of phytomining, a bio-based approach, to recover valuable metals from contaminated soils or used batteries using hyperaccumulator plants. The concept of phytomining synergizes with the bioresource-focused research, as it aligns with the sustainable utilization of plants for resource recovery. This approach contributes to responsible sourcing of metals required for energy storage technologies. In summary, the production of nanocellulose and graphene from EFBs and palm oil waste, alongside the innovative concept of phytomining, exemplifies the power of biomass innovation and circular economy in transforming waste and sustainable resource into valuable resources, driving economic growth, and fostering a sustainable bioeconomy. By harnessing the potential of biomass and sustainable resource, more efficient, resourceful, and environmentally friendly future can be created.

*Keywords: nanocellulose, graphene, biomass, circular economy, phytomining*

## Miniaturized Tubular Devices for the Wireless Separation of Racemic Mixtures

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### Abstract

Bipolar electrochemistry (BPE) is a powerful tool to induce a pumping effect in conducting polymers [1] without the need of further physical connections. Recently we have introduced an additional functionality to the wireless electropumping, *i.e.* enantioselectivity, functionalizing polypyrrole tubes with inherently chiral oligomers [2]. The synergy between the electromechanical properties of polypyrrole and the enantiorecognition features of inherent chiral oligomers leads to the enantioselective loading and pumping of chiral analytes [3].

In particular, in the present work, we have successfully tested either racemic or unbalanced mixtures of chiral analytes released by our hand-made chiral tubes analyzing the collected fractions with chiral HPLC, in order to verify the separation efficiency of our systems.

The difference in retention time between the antipodes of the chiral molecule under study, will allow the possible applicability of these miniaturized enantioselective devices in chiral separation techniques.

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**Keywords:** Chirality, Polypyrrole, Separations, Enantioselectivity, Miniaturized Devices

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## Bifunctional hafnium-isomorphously substituted Beta zeolite for one-pot 5-hydroxymethylfurfural synthesis from glucose

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### Abstract

5-hydroxymethylfurfural (HMF) has been one of the most crucial bio-based building blocks for producing biobased monomers in biorefineries. Typically, it can be produced from glucose via consecutive steps of glucose isomerization and fructose dehydration. Recently, the synthesized zeolites containing Brønsted acid and Lewis acid properties have been applied as outstandingly active and selective catalysts due to their unique acid properties and their confinement effects to produce a desired product selectively. For instance, Sn-incorporated zeolites exhibit efficient catalytic activity due to the distinct Lewis acid strength, eventually promoting glucose isomerization[1]. With the co-existing Brønsted acid properties stemming from tetrahedrally-coordinated Al species in silica matrices, the following fructose dehydration is able to be selectively triggered. However, isomorphously-substituted Sn species feature low stability in the reaction media, leading to a restructuring of the active species or an expulsion from the zeolite matrices[2]. In this contribution, we demonstrate the first example of the rational design of bifunctional hafnium-isomorphously substituted Beta zeolites. The introduction of the isolated Hf species into aluminosilicate matrices is achieved by the *in-situ* hydrothermal method, revealing the distinct Lewis acid and Brønsted acid properties. Their relatively high reactivity results from their increased ability to accept an electron from acyclic glucose during rate-determining hydride transfer of glucose isomerization reaction, compared to the well-known Sn-incorporated zeolites, as evidenced by DFT calculations. While the typical Sn-incorporated zeolite not only promotes HMF production but also shows its high activity in producing an undesired product. Most importantly, the isolated Hf species in zeolite frameworks feature long-term stability under reaction-regeneration conditions. In contrast, the deactivation of the Sn-containing zeolite is obtained due to the transformation of Sn active species and the formation of leached Sn species in the reaction medium[3].

**Keywords:** 5-hydroxymethylfurfural, glucose, hafnium-beta zeolites, heterogeneous catalysis

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# Synthesis and characterization of copper-based metal-organic frameworks

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## Abstract

This work has studied efficient, non-toxic, and scalable copper-based metal-organic frameworks (MOFs), which are an ideal structure for carbon dioxide capture. The characterization was carried out using FTIR, XRD, SEM, BET, and TGA techniques. FTIR results showed the presence of terephthalic acid at  $1662\text{ cm}^{-1}$  as a carbonyl functional group, revealing the presence of benzene dicarboxylic acid (BDC)-based MOFs sites. XRD results exhibited that MOFs have a cubic crystal structure and a high-purity phase. Their thermal property was also confirmed by TGA, the results showed that the synthesized material could be applied at temperatures up to  $310\text{ }^{\circ}\text{C}$ . Moreover, in SEM images, it was found that the MOFs showed square-like shapes with a well-distributed size. The BET surface area was  $117.5\text{ m}^2/\text{g}$ , the pore volume was  $0.074\text{ cm}^3/\text{g}$ , and the average particle size was around  $50\text{ nm}$ . Furthermore, the BET surface area was compared with the other work using the same precursors of copper terephthalate and nickel terephthalate, showing that the surface area of the MOFs in this work is 23.23% and 70.46% higher than those, respectively. It can be concluded that they have a sufficient surface area to be used as an adsorbent or for gas separation due to their high surface area and porous structures.

*Keywords: copper-based metal-organic frameworks, absorbent, and carbon dioxide capture*



# Halloysite Nanotubes in Electrochemical Enantioselective Discrimination

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## Abstract

Halloysite nanotubes (HNTs), a clay mineral of the kaolin group, are composed of aluminosilicate layers with an external tetrahedral silica and internal octahedral alumina sheets. The hollow tubular shape, which is formed by the clay layers, is endowed with spiral-like morphology. Commonly, the length of these objects is found in the micrometer range, with an external and internal diameter between 60-300 nm and 10-60 nm, respectively. HNTs have attracted considerable attention due to their unique features such as biocompatibility, low-cost, surface reactivity, hollow cavities, easy dispersibility and high stability in different solvents. Nowadays, the development of novel and so far unexplored flexible substrates that can be used as cost-effective electrode materials for enantioselective applications is still challenging. In this work, we take advantage of the physico-chemical properties of HNTs, in order to use them as electrode substrates for the enantiorecognition of chiral probes guided by inherently chiral oligomers. A ceramic glassy carbon screen-printed electrode modified with HNTs (HNTs-SPE) was used for the potentiodynamic characterization of L- or D-3,4-dihydroxyphenylalanine (L- or D-DOPA). The voltammograms exhibit an improved current amplitude compared to the bare SPE electrode, corroborating an increase of the electrode active surface. Finally, for the case of the HNTs-SPE modified with the enantiomers of an inherently chiral oligomer, a differentiation between the two antipodes of DOPA in terms of current amplitude was observed. These results display the perspective to use HNTs modified electrodes as a new class of a chiral device opening up potential applications in the field of enantioselective recognition.

*Keywords: Halloysite nanotubes, Inherently chiral molecules, Analytical probes, Enantioselective recognition, Conducting polymers*

# Unlocking the Full Potential of Heteroatom-Doped Graphene-Based Supercapacitors through Stacking Models and SHAP-Guided Optimization

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## Abstract

Graphene-based supercapacitors hold significant promise as a cost-effective and high-capacitive performance for energy storage solutions. Heteroatom-doping is an alternative method for enhancing the capacitive abilities of graphene-based electrodes and performing at the optimal doping condition is essential for unlocking the electrode's performance. However, the optimal doping conditions and the significant electrochemical properties remain an ongoing challenge due to the synergistic effects that occur. The capacitance (CAP) of graphene-based electrodes can be affected by many factors, including % doping of element content, defects, specific surface area (SA), electrolyte, and more. In this study, we applied machine learning models to observe a suitable model for CAP prediction based on the analyzed data, the machine learning models include Light Gradient Boost Machine, Extreme Gradient Boost, Polynomial Regression, Neural Network, Elastic Net, Lasso Regression, Ridge Regression, Random Forest, Support Vector Machine, K-Nearest Neighbors, Gradient Boost, AdaBoost, and Decision Tree. Moreover, we aimed to identify the most accurate predictive model by taking advantage of the top candidate model and creating a stacking concept called "stacking models". Additionally, SHAP values were utilized to identify the critical properties influencing CAP, and it was discussed in more detail. Results show that a large SA, with approximately 4–5% nitrogen, 10–15% oxygen, high percentages of sulfur, a defect ratio close to 1, with acid electrolyte, and a low current density tends to obtain the high-capacitive abilities graphene supercapacitors. We expected that the developed model could be used as a valuable computational tool for future electrochemical research that applies from fundamental to applications.

*Keywords: Supercapacitor, Graphene, Two-dimensional Materials, Nitrogen, Machine Learning*

## Effect of Nanosized Cu-MOR Zeolite in Catalytic Dehydrogenation of Ethanol to Acetaldehyde

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### Abstract

Ethanol conversion is one of the promising alternative routes for the production of versatile chemicals, for example, acetic acid, ethylene, acetaldehyde, and diethyl ether. Among them, acetaldehyde is one of the vital chemicals to produce several industrial substrates, such as drugs, perfumes, and disinfectants. However, acetaldehyde production via the oxidative dehydrogenation still suffers because it requires the addition of oxygen under high temperatures, high production cost, and unfriendly environmental conditions. Therefore, non-oxidative dehydrogenation of ethanol to acetaldehyde is considered to be an alternative route. Indeed, several catalysts including metal oxides, zeolite, and mesoporous silica combined with noble metal active sites have been applied as promising catalysts. Although they performed high ethanol conversion, low acetaldehyde yield was obtained. In this contribution, we fabricated nanosized Cu-based mordenite (MOR) zeolites for ethanol conversion to acetaldehyde. The nanosized MOR zeolite was synthesized via a simple hydrothermal method using nano-silica as a silica precursor. Subsequently, the Cu-MOR was prepared via the ion-exchange method using Cu aqueous solution at the optimized conditions. The catalytic performance of dehydrogenation of ethanol to acetaldehyde was investigated using a fixed-bed reactor at 300-450°C. The reaction mixtures were analyzed using gas chromatography (GC) equipped with an FID detector and PoraBOND Q column. We reported here the catalytic performance of ethanol dehydrogenation to acetaldehyde over Cu-based nanosized MOR as displayed in Figure 1. It was found that the unmodified Cu-MOR with 4.5 wt% of Cu (4.5wt% Cu-MOR) provides 67% of ethanol conversion and 50% acetaldehyde yield. This work highlights new possibilities for acetaldehyde production from ethanol using the modified nanosized MOR catalyst.

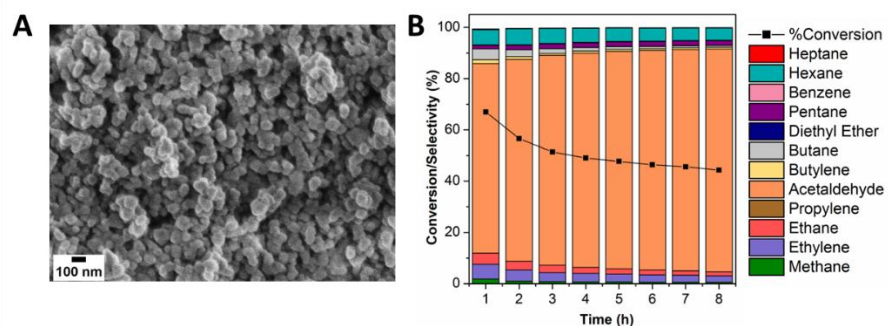


Figure 1. (A) SEM image and (B) Catalytic performances of 4.5wt% Cu-MOR for non-oxidative dehydrogenation of ethanol to acetaldehyde under the optimized conditions.

**Keywords:** MOR zeolite, Cu-based catalyst, Ethanol, Dehydrogenation, Acetaldehyde

# Effect of Surface Oxygen on the Dehydrogenation of Ethanol to Acetaldehyde over Isolated Zn Sites Supported on Dealuminated BEA Zeolite: A Computational Study

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## Abstract

The effect of surface oxygen on isolated zinc supported on dealuminated BEA zeolite (Zn-DeAlBEA) for ethanol dehydrogenation to acetaldehyde was investigated using density functional theory (DFT) with the M06-L method and coupled cluster [CCSD(T)] calculations. The reaction was proposed to proceed in two steps, the ethanol O-H bond dissociation and the ethoxide intermediate decomposition into acetaldehyde product. The activation free energy for the first step is 3.7 kcal/mol when using the ZnO-DeAlBEA zeolite, which is four times lower than the 12.1 kcal/mol obtained with the Zn-DeAlBEA zeolite. For the second step, the reaction barriers are 16.6 kcal/mol for ZnO-DeAlBEA and 34.4 kcal/mol for Zn-DeAlBEA, respectively. The results indicate that the presence of surface oxygen at the Zn site enhances both the dissociation of the ethanol O-H bond and the conversion of ethoxide to acetaldehyde, thereby boosting catalytic activity.

**Keywords:** *Biomass; Ethanol dehydrogenation; Acetaldehyde; Dealuminated zeolite; DFT*

# Catalytic Dehydroisomerization of Butane to Isobutene over Zeolite Composites

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## Abstract

The predominant industrial process for isobutene production as a fuel additive is steam cracking or catalytic cracking; however, it often suffers from a low yield of isobutene with a huge amount of emitted greenhouse gases. To overcome these issues, a novel strategy based on the dehydrogenation of n-butane, which is an endothermic reaction, and butene isomerization with an exothermic feature has been extensively explored. Nevertheless, they are facing high operating costs, the fast catalyst deactivation, and the large amount of by-products. Herein, we report the alternative way to rationally design zeolite composites containing as the core-shell structures of different zeolite frameworks for isobutene production in a single process via n-butane dehydroisomerization. For example, the FER/MFI zeolite composite was successfully fabricated by preliminary recrystallization of MFI nanocrystals at the external FER surface, followed by the further growth of the hierarchical structure of MFI, eventually producing the core-shell structure of FER as a core and MFI as a shell. To achieve the high dispersion of hydrogenation sites on a zeolite support, the PtZn incorporated on FER/MFI composite was prepared and they exhibited high catalytic performance in n-butane dehydroisomerization compared to the one containing the PtZn loaded on the bare FER or MFI (17.3% and 2.6% isobutene yield over the PtZn-FER/MFI and the PtZn-FER, respectively). The reason for the improved catalytic activity of the composite relates to the fact that the shell hierarchical MFI could be used to disperse PtZn species, eventually forming small PtZn nanoparticles, which are advantageous for alkane dehydrogenation to alkene [1]. Besides, the excessive acidity of the core FER in composite was suppressed [2] and this would facilitate the conversion of produced butene to isobutene simultaneously. In contrast, the insufficient metal dispersion on the bulk FER surfaces of the isolated FER (PtZn-FER) led to the formation of agglomerated PtZn particles which were ineffective in butane dehydrogenation. Moreover, the excessive acidity of PtZn-FER enabled the catalytic cracking of butene, resulting in low isobutene yield. This example opens up the perspective of the rational design of zeolite composites with fine-

## Tailoring ETL/ERI Zeolite Interfaces using Renewable Silica Source for Bio-Ethylene Production

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### Abstract

Hierarchical zeolites with intergrowth structures have exhibited many advantages over pure zeolites or physical mixtures in terms of catalytic, sorptive, or molecular separation properties.<sup>1,2</sup> However, the development of the well-defined zeolite with intergrowth structures is still in an early stage and it often suffers from the competition of phase separation of several metastable polymorphs.<sup>2</sup> In addition, phase competition leads to defect generation, and these defects can promote a different crystalline structure formation, referred to as intergrowths.<sup>3,4</sup> Herein, we demonstrate the synthesis of intergrowth zeolite of unique ETL and ERI frameworks by using a renewable silica source. In addition, the structural evolution of interfaces in ETL/ERI intergrowth zeolites has been successfully obtained. Finally, the perspectives of catalytic activity using ETL/ERI intergrowth zeolites in bioethanol dehydration to ethylene have been demonstrated. The different forms of ETL zeolite were obtained using various silica sources under both dynamic and static crystallization processes. For example, pure ETL zeolite is obtained using commercial colloidal silica (CSi), whereas changing silica sources to renewable nano-silica particles (NSP) results in the formation of the ETL/ERI intergrowth zeolite. The reason for the different phase formation relates to a different rate of hydrolysis and condensation between CSi and NSP. For example, in the static mode, the amorphous was obtained after 1 day of crystallization time (CT), while the crystalline ETL/ERI intergrowth zeolites were obtained after 2 days of CT when applying with NSP as a silica source. After prolonging the CT, a maximum ERI content (21 RC%) was obtained at 6 days of CT. A combination of XRD, TEM, and ED results confirms that ETL/ERI interfaces exist, possibly derived from competitive ETL and ERI crystal formation (Figure 1).<sup>3,4</sup> The designed intergrowth ETL/ERI zeolites show high ethylene selectivity (96 %) from bioethanol dehydration, whereas this situation cannot be achieved when using pure ERI. This work opens up the perspectives of intergrowth zeolites for catalytic applications.

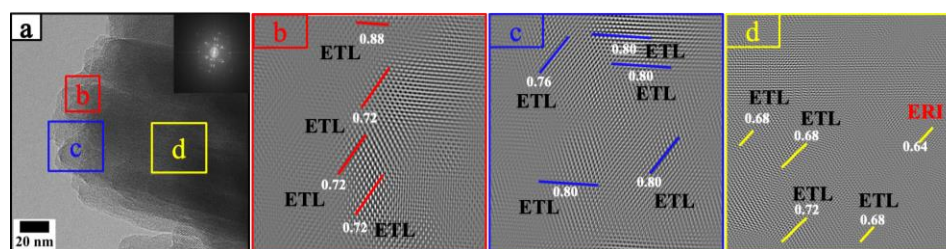


Figure 1. HR-TEM images of ETL/ERI intergrowth zeolite with respect to its Fast-Fourier Transform (a) and (b-d) the corresponding invert-FFT of the selected area images showing ETL and ERI phases.

**Keywords:** Intergrowth, Zeolite synthesis, ETL, ERI

## Effect of zeolite framework on the efficiency of implanted Ti active sites for methyl oleate epoxidation

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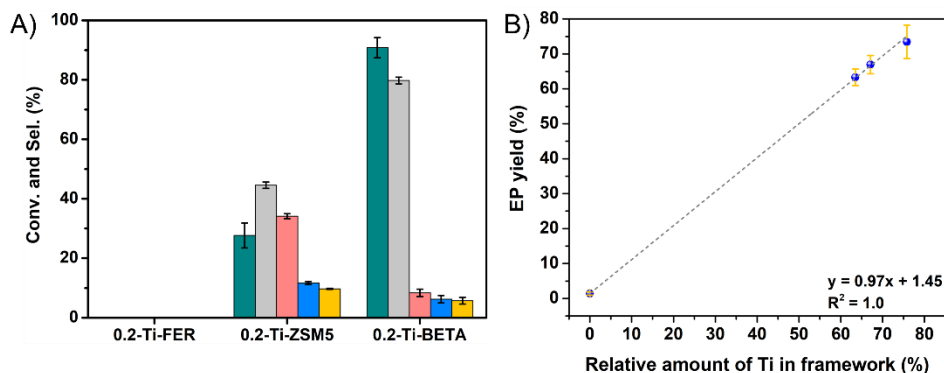
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### Abstract

The development of isomorphically substituted transition metals, especially the Ti atom, in a zeolite framework is one of the most promising perspectives for Lewis acid catalysis. In this contribution, we demonstrate the effect of the zeolite framework on the efficiency of incorporated Ti active sites in different zeolite topologies, such as MFI and BEA. It is observed that the zeolite framework can affect the structure of embedded Ti active species, confirmed by the UV-Vis DRS technique. The isolated tetrahedrally coordinated Ti active species has been successfully incorporated into the BEA zeolite framework (Ti-BEA). In contrast, the ZSM5 (MFI) framework primarily composes of tetrahedrally polymeric Ti species. To demonstrate the effect of the zeolite framework on the catalytic performance in methyl oleate epoxidation, the isolated tetrahedral Ti active sites in the BEA framework show superior catalytic activity in terms of methyl oleate conversion and epoxide selectivity compared to polymeric tetrahedral Ti-containing in ZSM5 zeolite (Ti-ZSM5). Noticeably, the product distribution obtained from Ti-BEA and Ti-ZSM5 catalysts is completely different. These observations relate to the fact that the differentiation of the electronic property of Ti active species could be obtained when incorporating in the different zeolite framework, eventually changing the catalytic activity of the catalyst.



**Figure 1.** A) the catalytic activity of the as-synthesized catalyst; MO conversion (green), selectivity of EP (gray), MDI (pink), MOX (blue), NN (yellow), and B) the relationship between EP yield and the relative portion of Ti I the zeolite framework.

**Keywords:** Zeolite topology, Ti species, and methyl oleate epoxidation

# CO<sub>2</sub> Transformation to MWCNT via Chemical Vapor Deposition Using Metal-Supported on Hierarchical Zeolite Template

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## Abstract

The pressing imperative to combat climate change has driven innovative research to mitigating carbon dioxide (CO<sub>2</sub>) emissions. A promising approach involves the conversion of CO<sub>2</sub> into valuable substances, particularly carbon nanotubes (CNTs), emerging as a versatile material for various technologies. This study introduces the novel concept of utilizing CO<sub>2</sub> to produce high-value-added CNTs, achieved through the utilization of metal-supported hierarchical zeolite catalysts. We have successfully developed Fe and Ni nanoparticles supported on hierarchical FAU and hierarchical ZSM-5 zeolites (HieFAU and HieZSM-5) via the impregnation method. Among these catalysts, the 25wt%FeHieFAU catalyst exhibited the highest yield for CNTs synthesis under the conditions of 800°C and a pressure of 5 barg with CO<sub>2</sub>. The resulting 15.4% CNTs yield was obtained using the 25wt% FeHieFAU catalyst and displayed remarkable characteristics, including a diameter size of 23.1 nm and an ID/IG ratio of 0.56, indicative of their exceptional quality. Moreover, the synthesized CNTs were subjected to electrochemical performance evaluation, demonstrating their superiority over commercial CNTs when employed with a 0.5 M H<sub>2</sub>SO<sub>4</sub> supporting electrolyte in cyclic voltammetry experiments (compared to Ag/AgCl). This superior current response, offered by these small-diameter and high-quality CNTs, underscores the potential advantages in their application in electrochemical technologies. This research paves the way for exploring new possibilities in utilizing CNTs to tackle CO<sub>2</sub>-related challenges and to technologies advancements in the electrochemical technology.

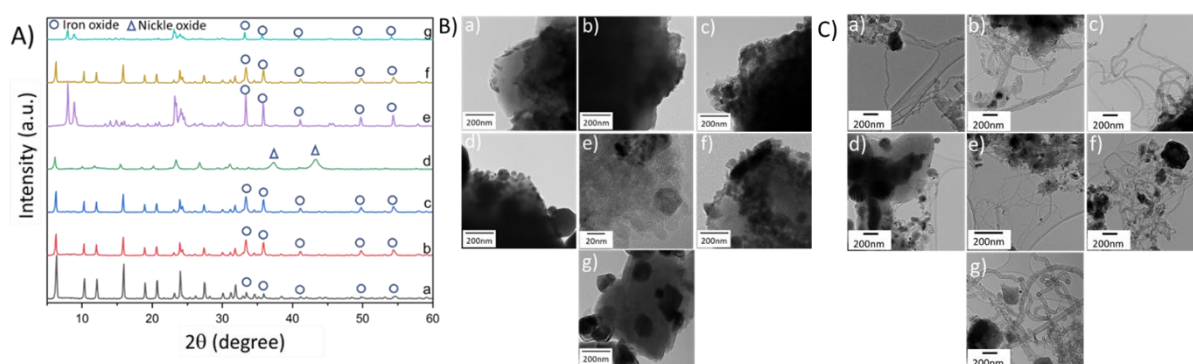


Figure 1. Characterization of transition metals supported by HieFAU and HieZSM-5 with various metal contents: A) XRD patterns and B) TEM image of a) 15wt%Fe-HieFAU, b) 25wt%Fe-HieFAU, c) 35wt%Fe-HieFAU, d) 25wt%Ni-HieFAU, e) 25wt%Fe-HieZSM-5, and f) 25wt%Fe-FAUCOM, g) 25wt%Fe-ZSM-5COM. B and C) TEM images of the synthesized CNTs obtained via a CCVD technique by using: a) 15wt%Fe-HieFAU, b) 25wt%Fe-HieFAU, c) 35wt%Fe-HieFAU, d) 25wt%Ni-HieFAU, e) 25wt%Fe-HieZSM-5, f) 25wt%Fe-FAUCOM, and g) 25wt%Fe-ZSM-5COM, respectively.

**Keywords:** CO<sub>2</sub> conversion, carbon nanotubes, transition metals, zeolite catalysts, electrochemical applications



# Insights into the Hydrolysis of Organophosphates from Theoretical Calculations

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## Abstract

Herein, we investigate the reaction mechanisms of P=O bond hydrolysis in various organophosphates using density functional theory calculations. We first examine the possible mechanisms of hydrolysis, namely concerted and stepwise, using paraoxon as a model at the M06-L/def2-TZVP level of theory. In the stepwise mechanism, nucleophilic water substitution at the phosphorus center takes place in two steps, leading to the elimination of the leaving group, while the concerted mechanism occurs in a single step without intermediate formation. The rate-determining step barrier for the stepwise mechanism, involving the initial attack of water oxygen on phosphorus and the transfer of a proton from water to the oxygen of the P=O bond, is 37.7 kcal/mol. This barrier is approximately 20 kcal/mol lower than the barrier of the concerted mechanism, which is 58.1 kcal/mol. Due to the smaller activation barriers associated with the stepwise pathway, it appears to be more favored than the concerted one. We evaluate the precision of M06-L in determining stepwise rate-determining barriers by comparing it to the DLPNO-CCSD(T) method with a complete basis set. Our results demonstrate that the barrier computed with M06-L closely aligns with the one obtained through DLPNO-CCSD(T) (37.7 vs 38.6 kcal/mol), affirming its accuracy for this reaction. Finally, we calculate the hydrolysis of various organophosphates and correlate the obtained barriers with energetic descriptors, including adsorption energy, intermediate energy, and the energy difference between intermediate and adsorption. We observe a strong relationship between the barrier and the intermediate energy with an  $R^2$  determination coefficient of 0.81. Consequently, intermediate energy is proposed as a descriptor for approximating the activation barrier without the need to locate the transition state.

**Keywords:** *Organophosphate; Hydrolysis; Reaction Mechanism; DFT*

# Density Functional Investigation of the Carbon Dioxide Capture over Glycine-Functionalized Metal-Organic Frameworks

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## Abstract

Here, we employ density functional theory (DFT) calculations to investigate the reaction mechanism of carbon dioxide (CO<sub>2</sub>) capture on glycine-functionalized metal-organic frameworks-808 (MOF-808). To determine the geometrical structures and energetic properties along the reaction coordinates, we use the M06-L density functional with the def2-SVP basis set for the C, O, H, and N atoms, and the LANL2DZ basis set for the Zr atom. To investigate the effect of glycine functionalization, we treat MOF-808 with 1, 2, and 4 glycine molecules. The reaction is assumed to be a single step in which the proton of the glycine amino group transfers to the oxygen of CO<sub>2</sub>, and simultaneously, the C-N bond is formed to produce the carbamate. The reaction barriers for the functionalization of MOF-808 with 1, 2, and 4 glycine molecules are 47.2, 45.7, and 43.6 kcal/mol, respectively. The relative energies for carbamate formation during the functionalization of MOF-808 with 4 glycine molecules are -13.5 kcal/mol, which is higher than those for 1 (-4.8 kcal/mol) and 2 (-11.8 kcal/mol) molecules. These results indicate that as the number of glycine molecules used for functionalization on MOF-808 increases, the CO<sub>2</sub> capture performance also increases. We also study the capture reaction under humid conditions by introducing an explicit water molecule. We observe that the presence of a water molecule resulted in reduced barriers for glycine substitutions at all levels and greater stability in carbamate formation, indicating a higher performance of glycine-functionalized MOF-808 for CO<sub>2</sub> capture.

**Keywords:** Carbon dioxide; Capture; Metal-organic frameworks; DFT

# Chiral-Induced Spin Selectivity Effect at Chiral-Encoded Pt-Ir Surfaces for Enhanced Oxygen Reduction Reaction

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## Abstract

The Chiral-Induced Spin Selectivity (CISS) effect has been recently proposed as an interesting concept for many different applications. In particular, it has a significant impact on the oxygen reduction reaction (ORR), which plays an important role in clean energy production such as with fuel cells, due to the high electron transfer efficiency from chiral electrode surfaces to oxygen molecules. To date, this perspective is still in an early stage of development, and it has been mostly investigated for electrodes modified with chiral organic monolayers or chiral assemblies. However, it has not been reported so far that a similar effect can also be achieved with intrinsically chiral metal surfaces without chiral monolayer adsorption. Recently, we have successfully developed chiral imprinted Pt-Ir alloys with mesoporous features by electrodeposition of metal salts in the simultaneous presence of non-ionic surfactants and various chiral compounds such as the enantiomers of phenyl ethanol. These designer materials can perfectly retain molecular chiral information, even after template removal. This allows using them for various applications such as asymmetric synthesis of chiral compounds and enantioselective analysis. In this contribution, chiral imprinted mesoporous Pt-Ir has been studied as an electrocatalyst for ORR. We show that such electrodes can significantly improve ORR due to the CISS effect, eventually leading to higher current intensities. However, this effect cannot be observed when using an achiral electrode of analog composition or which has been imprinted with the opposite enantiomer. This work opens up novel perspectives for developing catalysts for ORR based on the CISS effect, promoted at intrinsically chiral metal surfaces.

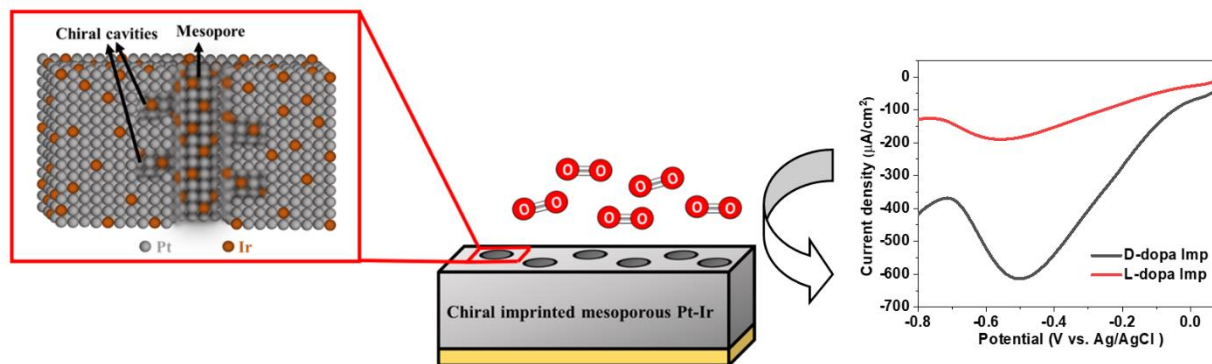


Figure 1. Illustration of the concept using a chiral imprinted mesoporous Pt-Ir electrode to promote ORR. Left: Scheme of the chiral imprinted alloy. Middle: Macroscopic chiral electrode. Right: Linear sweep voltammetry of two electrodes imprinted with opposite enantiomers in oxygen saturated electrolyte.

**Keywords:** electrocatalyst, oxygen reduction reaction, CISS effect

# Can Amine Ligand Atomically Disperse Cu Atoms on $\text{TiO}_2(110)$ ?: Cu Deposition on $\text{TiO}_2(110)$ Premodified With *O*-Anthranilic Acid

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## Abstract

Single-atom catalysts (SACs), which consist of isolated single metal atoms dispersed on oxide support, have recently attracted much attention due to their high catalytic activity and cost-saving of precious metals<sup>1</sup>. The SACs are usually obtained by immobilizing metal species on the oxide surface through the surface OH groups or linker molecules that strongly interact with the metal species and the support. However, the metal atoms are often aggregated to form particles particularly at high temperatures due to insufficient interaction between the metal atoms and the support surface, and the factors to control atomic dispersion are not well understood. Our group has developed the “premodified surface method” to obtain a highly dispersed metal species, where an oxide surface is precovered with a functional organic molecule possessing a substituent atom that can strongly coordinate to a metal atom<sup>2</sup>. Here, we used *o*-anthranilic acid (*o*-AA) as a surface-modified molecule to stabilize the single-atom Cu species. The three-dimensional structure of evaporated Cu atoms on a  $\text{TiO}_2(110)$  premodified with *o*-AA was examined using polarization-dependent total reflection fluorescence X-ray absorption fine structure (PTRF-XAFS) in three different polarized directions ( $E//[001]$ ,  $E//[1\bar{1}0]$  and  $E//[110]$ ) to elucidate the effects of the premodification on the Cu dispersion over the  $\text{TiO}_2(110)$  surface as shown in Fig.1. This work suggests that selecting a different functional molecule for premodification of a single-crystal  $\text{TiO}_2(110)$  surface enables fine-tuning of the coordination environment of surface Cu complexes. And the selection of a different linker molecule for premodification of a single-crystal  $\text{TiO}_2(110)$  surface offers a new strategy for fine tuning of the coordination environment around the atomically dispersed metal sites, which may lead to precise control of catalytic performances.

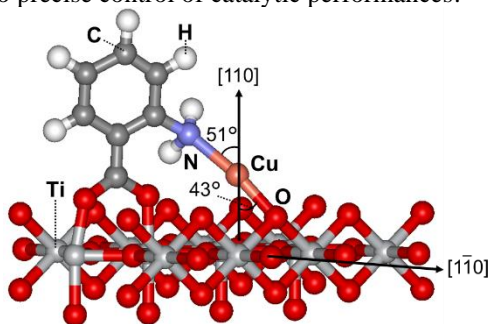


Fig. 1 Surface model structure of Cu on *o*-AA premodified  $\text{TiO}_2(110)$

**Keywords:**  $\text{TiO}_2(110)$ , premodified surface method, PTRF-XAFS

# Synthesis of Carbon-based Acid Catalysts from Lignin and its Activity toward Synthesis of Long-Chain Hydrocarbon Phase Change Material (PCM)

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## Abstract

In this study, lignin was used as a carbon source for catalyst preparation. Firstly, the lignin chars were prepared by the solvothermal reaction. In order to study the effect of types of lignin on the properties of the catalyst, two types of lignin were employed (i.e., commercial organosolv lignin (CL) and extracted bagasse lignin (EL)). The sulfonated carbon-based catalysts were then prepared. In order to study the effect of types of acid on the properties of the catalyst, two types of acid were carried out (i.e., sulfuric acid (SA) and methane sulfonic acid (MSA)). Several analytical techniques were carried out to characterize the lignin chars and catalysts.

The catalytic activities of synthesized catalysts toward the synthesis of phase change materials (PCMs) were studied. Various esters were synthesized to use as PCMs, and their thermal properties were investigated to determine the relationship between chemical structure and thermal properties. The results demonstrated that the increase of the carbon chain length of alcohol leads to a decrease in the phase change temperature and latent heat of the fatty acid ester. The melting temperature and latent heat of methyl stearate were 42.83 °C and 221.46 J/g, respectively. For comparison, the melting temperature and latent heat of ethyl stearate were 38.67 °C and 202.53 J/g, respectively. Moreover, the structure of fatty acid seems to have a higher impact on the phase change temperature of the resulting ester, compared to that of alcohol. Compared to the methyl stearate containing only carbon–carbon single bonds, the methyl oleate containing a single carbon–carbon double bond has a significantly lower melting temperature and latent heat (-10.9 °C and 163.13 J/g, respectively).

# Molecular Adsorption and Conversion at the Liquid/Solid-Oxide Interface by Computational Approach

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## Abstract

A comprehensive understanding of the interface between water and metal-oxide is fundamental due to its significance in a wide range of physicochemical phenomena and technological applications, such as catalysis, polishing, biomineral formation, colloid chemistry, and corrosion. The behavior of molecules at the water/metal-oxide interface is generally intricate, and probing the microscopic nature of the interface remains a formidable task for experimental methods. Molecular dynamics (MD) simulations offer a bottom-up picture of water/metal-oxide interfaces and have proven to be invaluable tools for the microscopic understanding of the structural properties and dynamical behaviors of water molecules at the interface.

In the first part of the talk, we will present some recent works on unique adsorption and catalytic reactions at the liquid/metal-oxide interface that are unveiled by the DFT-based MD simulations and advanced sampling techniques. In the second part of the talk, we will present our recent works using the neural network potentials (NNP). The NNP provides a reliable description of interatomic interactions for various types of bonding with high fidelity, and by efficiently acquiring and adaptively updating training data, usually obtained by the DFT calculations, the NNP-based MD simulations are becoming a versatile tool for investigating the microscopic structure and dynamical behavior of various systems with unprecedented system sizes and long simulation times.

*Keywords: DFT, neural network potential, molecular dynamics, cerium oxide, conversion*

**Short Bio: Akira Nakayama, Ph.D.**

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**Research Interests**

Our research group focuses on the development of computational tools for the microscopic understanding of the chemical processes based on the electronic structure theory, reaction dynamics, and statistical mechanics. We are primarily interested in the design of chemical reactions and materials related to environmental and energy issues.

**Education**

04/1998-03/2001	The University of Tokyo Ph.D. D., Department of Chemical System Engineering, Graduate School of Engineering
04/1996-03/1998	The University of Tokyo M.S. Department of Applied Chemistry, Graduate School of Engineering
04/1992-03/1996	The University of Tokyo B.S. Department of Applied Chemistry, School of Engineering

**Professional Appointment**

04/2019 – present	The University of Tokyo Professor, Department of Chemical System Engineering Graduate School of Engineering
10/2016 – 03/2020	Japan Science and Technology Agency (JST) PRESTO Researcher
10/2015 – 03/2019	Hokkaido University Associate Professor, Institute for Catalysis
07/2013 – 09/2015	Hokkaido University Associate Professor, Catalysis Research Center
10/2005 – 06/2013	Hokkaido University Assistant Professor, Department of Chemistry, Faculty of Science
10/2001 – 10/2005	University of Illinois at Urbana Champaign Postdoctoral Research Associate, Department of Chemistry
04/2001 – 09/2001	The University of Tokyo Postdoctoral Research Associate, Intelligent Modeling Laboratory

# Valorization of Biomass-Derived Chemicals and C1 Gases to Value-Added Commodities Via Catalytic Reactions

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## Abstract

Given the scarcity of fossil fuels and the increasing demand for renewable and sustainable energy sources, there has been a greater focus on converting biomass and C1 gas into valuable products. High fructose corn syrup, which is derived from biomass, stands out as the most affordable and readily accessible feedstock, making it highly promising for utilization as a source of monosaccharide. Catalytic conversion of glucose and/or fructose to 5-hydroxymethylfurfural (HMF) has gained considerable attention as an important precursor to produce high-value furanic chemicals, including 2,5-furan dicarboxylic acid (FDCA), tetrahydrofuran-2,5-dicarboxylic acid (THFDCA), 2,5-bis(hydroxymethyl)furan (FDM), 2,5-bis(hydroxymethyl)-tetrahydrofuran (THFDM), and more. FDCA has the potential to be used as a monomer for poly(ethylene 2,5-furan dicarboxylate) (PEF) when combined with ethylene glycol. Besides, FDCA can be converted to adipic acid via a two-step process with a 99% yield. It is worth noting that adipic acid has been recognized by International Energy Agency (IEA) as the most crucial dicarboxylic acid from an industrial perspective, mainly as a precursor for the production of nylon. When it comes to the utilization of C1 gases, our emphasis is on the production of dialkyl carbonates. Specifically, we are exploring an alternative approach for the production of dialkyl carbonates using CO and CO<sub>2</sub> gases, as opposed to the conventional method of hazardous phosgenation. Moreover, through the strategic application of bis(2-methoxyethyl) carbonate (BMEC) as a solvent for lithium salts, we have successfully addressed the fire hazards associated with the commonly used solvents, dimethyl carbonate (DMC) and diethyl carbonate (DEC), in Li-ion batteries. This advancement has been achieved while maintaining the desired level of ionic conductivity in Li-ion battery performance. Continued research for the development of innovative catalysts and reaction pathways will play a vital role in driving the production of renewable chemicals, fostering a greener and more sustainable chemical industry



## Short Bio:

**Jayeon Baek (백자연백자연), Ph.D.**

Senior Researcher

Areas of interest: Heterogeneous catalysis of C1 gas and biomass-derived chemicals

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## Experience

2018 - Present	Senior Researcher, Green and Sustainable Materials R&D Department, Korea Institute of Industrial Technology (KITECH)
2017 - 2018	Postdoctoral Scholar, Department of Chemical and Biomolecular Engineering, University of California, Berkeley (PI: Prof. Enrique Iglesia)
2015 - 2017	Postdoctoral Scholar, Department of Chemistry, University of California, Berkeley, Lawrence Berkeley National Laboratory (PIs: Prof. Gabor A. Somorjai and Omar M. Yaghi)
2015 - 2015	Postdoctoral Scholar, Institute of Chemical Processes, Seoul National University
2009 - 2015	Research Assistance, School of Chemical and Biological Engineering, Seoul National University
2009 / 2012	Teaching Assistance, School of Chemical and Biological Engineering, Seoul National University

## Education

2009 - 2015	Doctor of Philosophy, School of Chemical and Biological Engineering Seoul National University, Republic of Korea (PI: Prof. Jongheop Yi)
2005 - 2009	Bachelor of Science, Department of Chemistry, Ewha Womans University, Republic of Korea

## PUBLICATION - Peer Reviewed Journal

1. J. Lee†, A. -R. Jeon†, H. J. Lee, U. Shin, Y. Yoo, H. -D. Lim, C. Han, H. Lee, Y. J. Kim, J. Baek\*, D. -H. Seo\*, M. Lee\* “Molecularly engineered linear organic carbonates as practically viable nonflammable electrolytes for safe Li-ion batteries” *Energy & Environmental Science* (2023), Accepted (Cover featured)
2. H. J. Lee†, T. T. Nguyen†, A. V. Tran, H. S. Kim, Y. -W. Suh, J. Baek\*, Y. J. Kim\* “Engineering pKa value of 3 amine for enhanced production of dialkyl carbonate via Se-catalyzed oxidative carbonylation” *Journal of Industrial and Engineering Chemistry* (2023), 123, 140-149
3. A. V. Tran†, S.-K. Park†, H. J. Lee, T. Y. Kim, Y. Kim, Y.-W. Suh, K.-Y. Lee, Y. J. Kim\*, J. Baek\* “Efficient production of adipic acid by a two-step catalytic reaction of biomass-derived 2,5-furandicarboxylic acid” *ChemSusChem* (2022) (Cover featured)
4. A. V. Tran, H. J. Lee, J. H. Baik, J. Baek\*, Y. J. Kim\* “Montmorillonite K30 supported tungstophosphoric acid as an efficient catalyst for condensation reaction of methyl N-phenylcarbamate for generating diurethane” *Catalysis Letters* (2021) 152, 2206-2214
5. A. V. Tran, T. T. Nguyen, H. J. Lee, J. Baek, Y. J. Kim “An escape from noble metals for generating urethanes via reductive carbonylation of nitroarenes over FeSe<sub>2</sub>/γ-γ-Al<sub>2</sub>O<sub>3</sub>” *Catalysts* (2020) 10, 1228
6. C. C. Truong, Anh Vy Tran, T. T. Nguyen, J. Baek\*, Y. J. Kim\* “Azo-bridged Cesium salt of phenolate/triazolide as an unprecedented carboxylation catalyst for 1,3-disubstituted ureas from CO<sub>2</sub> and amines” *Advanced Sustainable Systems* (2020) <https://doi.org/10.1002/adsu.202000186>
7. D. K. Mishra, H. J. Lee, C. C. Truong, J. Kim, Y.-W. Suh, J. Baek, Y. J. Kim “Ru/MnCo<sub>2</sub>O<sub>4</sub> as a catalyst for tunable synthesis of 2,5-bis(hydroxymethyl)furan or 2,5-bis(hydroxymethyl) tetrahydrofuran from hydrogenation of 5-hydroxymethylfurfural” *Molecular Catalysis* (2020) 484, 110722
8. T. T. Nguyen, A. V. Tran, H. J. Lee, J. Baek\*, Y. J. Kim\* “Palladium-catalyzed reductive carbonylation of nitrobenzene for producing phenyl isocyanate” *Tetrahedron Letters* (2019) 60, 151310 (\*co-corresponding authors)
9. A. V. Tran, T. T. Nguyen, H. J. Lee, S. W. Bae, J. Baek, H. S. Kim, Y. J. Kim “CuSe<sub>2</sub>/CeO<sub>2</sub> as a novel heterogeneous catalyst for reductive carbonylation of nitroarenes for generating urethanes” *Applied Catalysis A: General* (2019) 587, 117245

# Unlocking Values in Biomass Toward Energy Transition

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<sup>a</sup> Department of Chemical Engineering, University of Louisville, KY

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## Abstract

The world's heavy reliance on petroleum, from plastic production to transportation fuels, contributes to climate change, hurting our food chain, living standards, and environment. In response to this challenge, lignocellulosic biomass emerges as a promising renewable carbon feedstock for producing advanced fuels and bioproducts in the bioeconomy. The transition to bioeconomy using biomass-derived alternatives offers compelling economic, societal, and environmental advantages. However, the inherent rigid chemical structure and limited accessibility of biomass to catalysts present obstacles to efficient conversion. Conventional biomass processing technologies often rely on high temperatures and/or pressures to enhance accessibility, resulting in elevated production costs, product degradation, and the formation of undesirable by-products. To establish a viable bioeconomy, we need to develop energy-efficient biomass processing technologies.

Our research team has addressed these challenges by developing innovative biochemical processes. In this presentation, we will elucidate the intricate structure-property relationship of biomass, which underpins the design of tailored biomass processing systems. These systems exhibit compatibility with biological pathways, enabling the efficient production of advanced fuels and bioproducts. Moreover, we will emphasize their role in advancing a circular bioeconomy and contributing to the critical mission of climate change mitigation, all while harnessing the potential of biomass feedstocks.

### **Short Bio**

Noppadon Sathitsuksanoh, Ph.D., is an Associate Professor in Chemical Engineering at the University of Louisville. His research group specializes in creating a biochemical toolbox for biomass conversion and carbon capture, focusing on polymer upcycling. Dr. Sathitsuksanoh is the recipient of the prestigious US National Science Foundation (NSF) CAREER Award for his innovative contributions to polymer upcycling. Additionally, he has been honored with the University of Louisville Trailblazer Award in recognition of the commercialization potential of his groundbreaking technology.

He serves as an Editorial Board Member for the Molecular Catalysis journal. He holds the position of Membership Chair for the Cellulose and Renewable Materials (CELL) Division of the American Chemical Society. Dr. Sathitsuksanoh's research and leadership contributions drive advancements in sustainable materials and renewable energy solutions.

## Solid biofuel and its future as an alternative energy source in Thailand

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### Abstract

Thailand is an agricultural country which produces various types of agricultural products such as rice, sugar, corn, tapioca flour, palm oil for domestic consumptions and exports. Hence, agricultural residues from these crops are generated in great numbers annually. Therefore, conversion of agricultural biomass to solid biofuel via torrefaction technology is considered as one of various alternative solutions for biomass valorization. This technology can enhance utilization of biomass more efficiently as promising sources of renewable energy. Thailand has acquired large numbers of coal for electricity generation and other industries during these past years. Considering the annual amount of unused agricultural residues, the solid biofuel generated from agricultural biomass has high potential for replacing coal consumptions in both electricity generation and industrial sectors. Therefore, the development of solid biofuel ecosystem with appropriate torrefaction technology in Thailand is a crucial and urgent agenda that needs to be addressed promptly and systematically for energy security and sustainability of the country.

*Keywords: Biomass, Solid biofuel, Renewable energy, Energy security, Sustainable ecosystem*

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**Profile**

A confident, diligent, and proactive researcher with great communication and spirituality for social integration

**Education**

- |                |   |
|----------------|---|
| 2018 – Present | Senior Researcher, National Nanotechnology Center (NANOTEC), National Science and Technology Development Agency (NSTDA), Pathum Thani, Thailand |
| 2013 – 2018    | Researcher, National Nanotechnology Center (NANOTEC), National Science and Technology Development Agency (NSTDA), Pathum Thani, Thailand        |
| 2008 – 2013    | Ph.D. Student in Materials Science and Engineering Department, Michigan Technological University (MTU), Michigan, USA                           |
| 2003 – 2007    | B.Sc. Student (2nd Class Honor) in Chemistry Department, Prince of Songkla University (PSU), Songkhla, Thailand                                 |

**Grant and Scholarship**

- |             |  |
|-------------|--|
| 2023 – 2024 | Funding from NRCT-EGAT in the topic of “Development of hydrogen production technology via dry reforming of biogas” as the principal investigator.  |
| 2020 – 2022 | Funding from Program Management Unit on Competitiveness (PMU C) in the topic of “Process development of high heating value biocoal production for biomass power plants” as the principal investigator. |
| 2017 – 2019 | Grant for New Researcher in the topic of “Design and development of mixed metal oxides catalysts for production of gamma valerolactone from biomass derivatives” from Thailand Research Fund (TRF)     |
| 2008 – 2013 | Royal Thai Government Scholarship in Science and Technology from Ministry of Science and Technology  |
| 2003 – 2007 | Science Achievement Scholarship of Thailand, Ministry of Science and Technology  |

# Revealing Kinetics Post Rate-Determining Step for Bronsted-Acid Catalyzed Reactions of Fructose

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## Abstract

The conversion of biomass feedstock into 5-hydroxymethylfurfural (HMF), a versatile platform chemical, has garnered significant attention as a source for sustainable chemical production. However, traditional methods for synthesizing HMF from sugars face inherent challenges, particularly when utilizing concentrated feedstock, resulting in undesired side reactions and low yields. Obtaining a deeper understanding of the sugar conversion mechanism for maximizing HMF yield presents a significant challenge due to the complexity of the reaction pathways, with most of the reactions being obscured by a few rapid rate-determining reactions.

This study investigates the impact of coexisting reactive species in the reaction, including glucose, fructose, HMF, and insoluble humins, on the homogeneous liquid-phase conversion of fructose to HMF. Variation experiments were carried out to establish correlations between the product distribution and key reaction parameters, including feedstock concentration, catalyst concentration, temperature, and reaction time. The resulting data were analyzed to yield a kinetic model that reliably explains the inverse relationship between sugar concentration in the feedstock and the HMF yield. Additionally, we demonstrate the plausibility of constructing a kinetic model for exploring post rate-determining reaction steps. This kinetic model served as the basis for a semi-batch reaction scheme, which led to a substantial improvement in HMF yield when compared to traditional batch synthesis using concentrated feedstock.

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### WORK EXPERIENCE

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#### Researcher

Aug 2020 – Present

*National Nanotechnology Center (NANOTEC), Thailand*

- Designed and developed lab-scale hydrothermal reactors for high-throughput kinetic studies
- Investigated in the effects of organic solvents on sugar dehydration reactions and developed a high-yielding, sustainable chemical process that resulted in a patent
- Developed a realistic kinetic model for sugar dehydration in organic solvents and used the model to design a chemical process that produced an unprecedentedly high product yield from a high feed concentration. (Patent and publication in preparation)
- Mentored an undergraduate student for his senior thesis that resulted in a publication on which he was a co-author

#### Graduate Research Assistant, Advisor: Prof. Matthew Neurock

Sept 2014 – June 2020

*University of Minnesota, Department of Chemical Engineering and Materials Science*

- Investigated in the effects of polar aprotic solvent on the acid-catalyzed dehydration of biomass using ab-initio molecular dynamics simulations
- Examined the effects of anions on the catalytic activities of acid-catalyzed sugar dehydration
- Analyzed the effects of reaction environment on the conversion rate and selectivity for the production of furan chemicals from sugars
- Developed an atomistic model that describes the localization of cations and active sites in aluminosilicate materials and their influences on the reaction mechanism of sugar isomerization and acid-catalyzed dehydration in presence of polar aprotic solvent

#### Undergraduate Research Assistant, Advisor: Prof. Paul J.A. Kenis

Jan 2012 – May 2014

*University of Illinois, Department of Chemical & Biomolecular Engineering*

- Developed microfluidic devices for biological applications that resulted in a publication
- Performed high-throughput antibiotics screening on multi-resistant pathogens using microfluidic devices

#### Intern

*National Nanotechnology Center (NANOTEC), Thailand*

July – Aug 2013

- Modified a synthesis process for a heavy metal adsorbent that increased the adsorption rate and capacity
- Constructed a lab-scale adsorption testing unit to determine the heavy metal adsorption capability

### EDUCATION

---

#### Ph.D., Chemical Engineering

Sept 2014 – 2020

*University of Minnesota, Twin Cities*

GPA: 3.62/4.00

#### B.S., *magna cum laude*, Chemical and Biomolecular Engineering

Aug 2010 – May 2014

*University of Illinois, Urbana-Champaign*

GPA: 3.83/4.00

### TECHNICAL SKILLS

---

#### Analytical Skills

- Chemical characterization: HPLC, GC-MS, UV-Vis, XRD, ATR-FTIR
- Microscopy techniques: Time lapse fluorescence, SEM, Phase contrast, DIC

#### Computational Skills

- Programing skills: Python and Bash programming languages
- Molecular simulations: CP2K, VASP, Gaussian, GROMACS
- Visualization tools: VMD, Origin, Google SketchUp, Adobe Illustrator

#### Microfabrication Skills

- Photolithography and soft lithography (microfluidic devices)
- Class 100 clean room experience

# Nanopores for Fingerprinting and Sequencing Individual Proteins

Cees Dekker<sup>a\*</sup>

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## Abstract

Nanopores are versatile biophysical sensors for single biomolecules. In the past decade, they even have been developed into a technology single-molecule DNA sequencing. New efforts are directed towards the fingerprinting and sequencing of proteins at the single-molecule level. In this talk I will present two examples of our recent research in this direction.

### 1. Trapping a single protein using a nanopore electro-osmotic trap (NEOtrap).

We developed a new type of single-protein trap, which we name nanopore electro-osmotic trap (NEOtrap). Here, an origami structure is used to create a strong electroosmotic flow in a solid-state nanopore, which allows us to catch a single protein and hold it at the most sensitive region of the nanopore for label-free sensing. This allows to distinguish various proteins, as well as study the dynamics of a single protein for a long time (even hours). Orientation control and linking of the DNA origami sphere can significantly improve the NEOtrap. Recent experiments on dCas9/RNA/DNA allow for modelling the trapping kinetics.

### 2. Nanopore-based sequential reading of individual peptides

We demonstrated [2] a nanopore-based single-molecule peptide reader that is capable of reliably detecting single amino-acid substitutions within individual peptides. A peptide is chemically linked to a DNA molecule and sequentially pulled through a biological nanopore by a DNA helicase in single amino-acid steps. Stepping ion-current signals enable discrimination of single-amino-acid substitutions in single reads. Notably, we demonstrated the capability to ‘rewind’ peptide reads, obtaining indefinitely many independent reads of the same molecule, yielding an undetectably low error rate in single-amino-acid variant identification.

Recently [3], we expanded this concept to discriminating post-translational modifications (PTMs). PTMs play a key role in regulating protein activity and they are the crucial elements underlying the enormous diversity in the proteome. Current mass-spectrometry detection methods cannot measure PTMs in single molecules or differentiate between closely spaced PTM sites. We demonstrated the ability to detect PTMs at the single-molecule level on immunopeptide sequences with cancer-associated phosphate variants by controllably drawing the peptide through the sensing region of a nanopore. We discriminate peptide sequences with one or two closely spaced phosphate PTMs with 95% accuracy for individual reads of single molecules. The data also prompted us to start modelling the traversal of peptides of mixed charge through nanopores. In my presentation I will present the state of the art of these experiments in our lab, which is expanding efforts to detecting a range of other PTMs and developing a workflow to read natural proteins.

These proof-of-concept experiments constitute a promising basis for the development of a single-molecule protein sequencer.

## References:

- [1] S. Schmid et al, Nature Nanotechn. 16, 1244 (2021); C. Wen et al, Nano Lett. 23, 3, 788 (2023)
- [2] H. Brinkerhoff, A.S.W. Kang, J. Liu, A. Aksimentiev, C. Dekker, Science 374, 1509 (2021)
- [3] I.C. Nova, J. Ritmeijeris, H. Brinkerhoff, T.J.R. Koenig, J.H. Gundlach, C. Dekker, Nature Biotechnology, DOI 10.1038/s41587-023-01839-z (June 2023).



# Transport Across Biological Nanopores

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## Abstract

Our team is interested in the transport of small molecules across channel forming membrane proteins. For example, how antibiotics enter Gram-negative bacteria, how to quantify the passage of small molecules across biological nanopores and what chemical scaffold facilitates the passage. On the other hand, we can also use channels for detection of biomarkers. For this we produce or engineer bacterial outer membrane proteins and reconstitute them in planar lipid membranes. The experimental requirement requires often small volumes, low noise and high stability for which no standard solution exists. I will outline the main experimental approaches to quantify the permeability of small molecules through nanochannel and potential applications.

## References

1. JD Prajapati U Kleinekathöfer, M Winterhalter. How to Enter a Bacterium: Bacterial Porins and the Permeation of Antibiotics. *Chem Rev.* 121 (2021) 5158-5192.
2. J Wang, Prajapati, F Gao, YL Ying, U Kleinekathöfer, M Winterhalter, YT Long. Identification of single amino acid chiral and positional isomers using an electrostatically asymmetric nanopore. *JACS* 144 (2022) 15072-15078.
3. Y Chen, A Barba-Bon, B Grüner, M Winterhalter, MA Aksoyoglu, S Pageni, M Ashjari, K Brix, G Salluce, Y Folgar-Cameán, J Montenegro, Werner M Nau. Transmembrane and Intracellular Delivery of Cationic Peptides Metallacarborane Cluster Anions of the Cobalt Bisdicarbollide-Type as Chaotropic Carriers for Transmembrane and Intracellular Delivery of Cationic Peptides. *JACS* 145 (2023)

**Short Bio:**

Mathias Winterhalter is Professor of Biophysics at Constructor University Bremen (formerly called Jacobs University) since 2003. He performed his PhD at the Freie Universität Berlin with W. Helfrich in 1988 and obtained his Habilitation at the Biozentrum Basel. From 1998-2003 he was Professor of Biophysics at the Université Toulouse Paul Sabatier (Institut Pharmacologie et Biologie Structurale, CNRS UMR 5089). From 2013-2018 he was Leader of the Managing Entity of Translocation, a subprogram of the ND4BB - Innovative Medicine Initiative platform devoted to understand and to provide tools with respect to the permeability barrier of the outer cell wall of Gram-negative bacteria.

Together with Prof Yi-Tao Long and Meni Wanunu we organize weekly webinars on Nanopore as a service to the Community: <https://sites.google.com/view/nanoporemeeting2020/weekly-meeting>.

# Nanopore Sensors for Single-Molecule Metabolite Sensing and Enzymology

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## Abstract

Biological nanopores are emerging as powerful tools for studying proteins at the single-molecule level. We show that proteins can be immobilized inside nanopores under the action of an electroosmotic flow, which generates from the directional flow of water across the nanopore. Proteins remain native-like and fully functional; and can be trapped for up to hours. The ionic current through the nanopore can then be used to measure conformational changes within the immobilized proteins.

We use this approach to measure the concentration of a wide range of metabolites binding to a range of different proteins. Importantly, metabolites can be detected with nanomolar sensitivity directly from complex biological samples. Since ionic currents can be easily interfaced with portable devices, this method is ideally suited for home-diagnostic, wearable or clinical devices. Furthermore, we found that nanopore currents can measure conformational changes with a resolution that largely surpasses other single-molecule methods, which revealed surprising new mechanisms on enzyme kinetics.

# Biological Nanopores: Their Roles in Nutrient Uptake and Antibiotic Transport and Their Implications in Novel Antimicrobial Agent Development

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## Abstract

Biological nanopores have immense implications in biotechnology and biomedicine. In Gram-negative bacteria, there are outer membrane porins that serve as biological nanopores that act as the molecular gateway not only for the entry of nutrients, but also antimicrobial agents. Therefore, the permeability of these molecules directly determined the cellular metabolism, as well as the survival rates of the bacteria. In our study, we first investigated the structure and function of BpsOmp38, which was a major outer membrane porin from the highly multidrug resistant *Burkholderia pseudomallei* and found that this protein channel was directly involved with the permeability of cephalosporin and cabapenem antibiotics. In the later work, we demonstrated a chitooligosaccharide-specific channel (so-called ChiP) from three highly pathogenic bacteria: *Vibrio harveyi* (VhChiP), *V. cholerae* (VcChiP), *Serratia marcescens* (SmChiP). VhChiP and VcChiP were classified as OmpC-like trimeric ChiPs, while SmChiP was a member of OprD like porin. Single channel electrophysiological data demonstrate that VhChiP formed a stable channel with a conductance value of  $1.8 \pm 0.3$  nS, while VcChiP was a highly fluctuating channel and voltage-dependent. On the other hand, SmChiP had a conductance value one-third of VhChiP ( $0.5 \pm 0.1$  nS), corresponding to the monomeric architecture of this protein. All three channels were selective towards chitooligosaccharides, the breakdown products of chitin by chitin processing enzymes secreted by each bacterial strain. In our recent study, we demonstrated that VhChiP and SmChiP could serve as the entrance for aminoglycoside antibiotics. In terms of applications, we carried out the chemical synthesis of chitooligosaccharide-based silica nanodots and these functionalized nanodots could block VhChiP channel strongly, which provide further prospective to develop powerful channel blockers based on functionalized nanomaterials that could provide the molecular basis for novel development of chitooligosaccharide-based antibiotics that could tackle *Vibrio* and *Serratia* infections.

**Keywords:** Chitooligosaccharide, SmChiP, VcChiP, VhChiP, antibiotic resistance.

**Funding sources:** National Research Council and Vidyasirimethi Institute of Science and Technology and National Research Council of Thailand

## Structural- and Surface- Modifications of Solid-State Nanopores for Active Ion Translocation Control and Sensing applications.

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Jakrapong Supadech<sup>c</sup>, Kittipong Tantisantisom<sup>a</sup>, Kawin Loha<sup>d</sup>, Ibrar Alam<sup>a</sup>,  
Harit Pitakjakpipop<sup>a</sup>, Albert Schulte<sup>d</sup>, Deanpen Japrun<sup>a</sup>

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<sup>d</sup> School of Biomolecular Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Rayong, Thailand.

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### Abstract

Nanopores have been known as powerful devices for single molecule detection of nucleotides, proteins, and biomolecules. Recently, solid-state nanopores have caught research interest as knowledge advance in material science and surface chemistry allows freedom of design strategy to modify the solid-state nanopore to match research requirements. In this talk, modifications of solid state nanopores are presented for specific applications. In one case, structural modification on nanopore is performed to gain active control of ionic current passing through the nanopore. Stack layers of metal and oxide are carefully and orderly selected to deposit on silicon nitride membrane, prior to the nanopore fabrication with focused ion beam, to obtain an electrode on the nanopore-rim. This metal contact is employed as a gate to manipulate electrical double layer within the nanopore through applied electric field. Parameters such as gate voltage, electrolyte concentration, pH, and pore size are varied to investigate ion translocation behavior under the influence of electric field. The finding could lead to the development of field-effect nanovalve for accurate control of ion/molecule translocation. On the other work, the nanopore structure and its side wall are modified for nucleotide sensing purpose. The probe molecule is designed to bind complementarily with the target nucleotide and is attached to the nanopore side wall by a gold-thiol chemistry. The modified nanopore shows significant conductivity change when the target molecules pass through the nanopore. This is attributed to the hybridization between the target nucleotide and the probe molecule. The results provide a potential approach for nucleotide sensing. In addition, our results show that the hybridization is reversible, allowing the reusability of the nanopores in multiple detection.

*Keywords: solid-state nanopore, field-effect nanopore, surface modification, electrical double layer, probe-nucleotide hybridization*

**Short Bio: Thitikorn Boonkoom**

Nanorobotic System and Nanoneedle Research Team (NRN),  
Responsive Material and Nanosensor Research Group (RMNS),  
National Nanotechnology Center (NANOTEC),  
National Science and Technology Development Agency, (NSTDA),  
Pathum Thani, THAILAND  
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**Education**

- |      |   |
|------|---|
| 2013 | Doctor of Philosophy (Chemistry)<br>Department of Chemistry, Faculty of Natural Sciences, Imperial College London, UK<br>Thesis: InP Quantum Dots for Hybrid Photovoltaic Devices                                 |
| 2008 | Master of Research in Nanomaterials<br>Department of Chemistry, Faculty of Natural Sciences, Imperial College London, UK<br>Dissertation title: Synthesis and Characterisation of Functionalised Quantum Dots for |
| 2006 | Bachelor of Science (Chemistry)<br>Department of Chemistry, Faculty of Science, Kasetsart University<br>Senior project: Synthesis of Nickel Microtube by Metal Reduction method                                   |

**Research experience**

Structural characterisation (X-ray Absorption Spectroscopy) and electronic characterisation (X-ray Photoemission Spectroscopy) using Synchrotron Light Radiations  
Workshop training on Synchrotron radiation beamline design and characterisation techniques, Chieron School  
2013, at SPring-8, JAPAN  
Schottky and Ohmic Contact Fabrication Training on silicon-based electronic devices at Thai Microelectronics Center (TMEC), THAILAND  
Synthesis of inorganic semiconductor nanoparticles (i.e., CdSe quantum dots, InP quantum dots, and ZnO nanowires) via solvothermal methods  
Photophysical characterisation using Transient Absorption Spectroscopy  
Fabrication and characterisation of photovoltaic devices and light emitting diodes  
Fabrication and characterisation of silicon-based nano/micro-scaled devices

**Proceedings and Publications**

1. L. Kittigul, J. Meephansan, P. Sirithanabadeekul, S. Hanvivattanakul, R. Deenonpoe, W. Yingmema, K. Tantisantisom, S. Thongma, Y. Rayanasukha, T. Boonkoom, P. Adulyariththikul, and P. Khanchaitit. The efficacy of LED microneedle patch on hair growth in mice. Archives of Dermatological Research, 2023, 315, 971-982.
2. P. Sornmek, D. Phromyothin, J. Supadech, K. Tantisantisom, and T. Boonkoom, Regulation of ionic current through a surround-gated nanopore via field effect control. Physical Chemistry Chemical Physics (2022), 24, 24866-24872.
3. S. Chanpraphan, T. Boonkoom\*, and R. Mathaapanon\*, Studies on nucleation and growth of Al<sub>2</sub>O<sub>3</sub> on polymer substrates using atomic layer deposition at low temperature, Proceedings of the Pure and Applied Chemistry International Conference 2020 (PACCON2020), 2020, 62-67
4. W. Thongkham, C. Lertsatitthanakorn, K. Jiramitmongkon, K. Tantisantisom, T. Boonkoom, M. Jitpukdee, K. Sinthiptharakoon, A. Klamchuen, M. Liangruksa, and P. Khanchaitit, Self-Assembled Three-Dimensional Bi<sub>2</sub>Te<sub>3</sub> Nanowire-PEDOT:PSS Hybrid Nanofilm Network for Ubiquitous Thermoelectrics, ACS Appl Mater Interfaces., 11 (6), 2019, 6624-6633
5. S. Thongma, K. Tantisantisom\*, N. Grisdanurak, and T. Boonkoom\*, UV enhanced White-light Response Based on p-Si/n-ZnO Nanorod Heterojunction Photosensor, Sensor Actuat A-Phys, 296 (2019), 324-330

# Large Cuozoan Pore-Forming Proteins as New Resources of Biological Nanopores

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## Abstract

Cubozoan or box jellyfish, is considered the most venomous creature on the planet. They are predominantly prevalent in tropical Indo-Pacific regions. Regarding the Thai DMCR and research team survey, a taxonomic investigation has identified 14 box jellyfish in Thai waters. The venom activity of two multi-tentacled box jellyfish species was investigated, and the proteomic approach was employed to define the protein components of the venom. Interestingly, considering hemolytic toxic effects are thought to be the fatal mechanism of box jellyfish envenomation, proteomic studies revealed that several of the detected proteins matched to pore-forming protein toxins (PFTs), the porin family, and hemolysin. Given the recent discovery of Cubozoan, a number of newly identified species have emerged. Consequently, their venoms remain mostly unexplored, harboring a plethora of intriguing bioactive peptides and toxins. These substances hold great potential as a novel source for possible biomedical and biotechnological applications.

**Short Bio:**



**Nuankanya Sathirapongsasuti, M.D., Ph.D.**

**Professional Affiliations and Activities:**

Thai Working Group on the Toxic Marine Animal

Secretary of the Expert Opinion Protocol Committee on jellyfish envenomation especially box jellyfish envenomation

Director of Research Network of NANOTEC, Translational Research In Nanotechnology based Diagnostics (TREND) 2018-2022

Reviewer of the Government Pharmaceutical Organization (GPO) Strategic Plan 2016-2020

**Research Experiences:**

**LECTURER, MAHIDOL UNIVERSITY; BANGKOK, 2013 - PRESENT**

I. Identify and study how microRNAs alter the expression of key genes involved in developmental and pathophysiology of human diseases

II. Multi-omics data integration to identify novel pathways in kidney diseases

III. Thai water box jellyfish: species identification, venom biochemistry and toxicological responses

IV. Translational research in nanotechnology-based diagnostics

**JUNIOR RESEARCHER, UNIVERSITY OF HAWAII AT MANOA; HAWAII, 2012 - 2013**

I. Discovery of nonrodent-borne hantaviruses using high throughput sequencing

**POSTDOCTORAL FELLOW, UNIVERSITY OF TOKYO; TOKYO, 2010 - 2011**

I. The differential expression of non-coding RNA in cancer cells under hypoxic condition

**Education**

MD

Faculty of Medicine Ramathibodi Hospital, Mahidol University, 2005

PHD

Department of Medical Genome Sciences, Graduate School of Frontier Sciences  
The University of Tokyo, 2010



## Southeast Asia Applied Science Hub “One CDC” Concept to Support Cross-CIO Collaborative Applied Science Activities that Accelerate Global Health Security (GHS)/Fund and Training Support

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### Abstract

Priority is given to activities that propose a “One CDC” approach to build up for pathogen discovery capacity by next generation sequencing (NGS), metagenomic NGS (mNGS), bioinformatics and epidemiology genetics to interpret and apply these data to inform public health policy maker or active surveillance purpose. CDC works closely with Thai National Institute of Health (NIH) and support CoAg funding for the Training center for Excellence in Medical Sciences (TEMS) to enhance laboratory workforce capacity with advance laboratory technologies nationally and regionally. Under the research hub, CDC Headquarter will encourage the subject matter experts (SMEs) to submit the proposal of research interest to work with Thailand partners in various sectors such as ministry of public health, national institute of health, academics and others in the related interested.

This year CDC has given award for Academic cooperative agreement (CoAg) with 2 universities in Thailand (Mahidol and Chulalongkorn university) that expand opportunity to the researchers in academic sectors to apply for the grant over the previous ministry of public health (MOPH) CoAg with allow only the researcher under the MOPH to apply for Research or Non-research projects.

**Short Bio: PONGPUN SAWATWONG, Ph.D.**

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Dr. Pongpun Sawatwong (Pii) received his PhD from Faculty of Tropical Medicine, Mahidol University. He is currently the deputy laboratory branch, Division of Global Health Protection Program. He also serves as the molecular lead focusing in advance molecular for infectious diseases especially for viral and bacterial Emerging or Re-emerging diseases including antimicrobial resistance by using next generation sequencing both short-read (Illumina) and long-read (Oxford Nanopore) platform. He has supported for NGS training in-country and SEA region including provide support NGS testing for ministry of public health.

**EDUCATION**

2011-2016	Ph.D. (Tropical Medicine), Mahidol University, Bangkok, Thailand
2005-2010	M.Sc. (Health Education and Behavior Sciences), Mahidol University, Bangkok, Thailand
1991-1995	B.Sc. (Medical Technology), Chiang Mai University, Chiang Mai, Thailand

**WORK EXPERIENCE**

2017-present	Medical Research Scientist/Deputy Laboratory branch chief. Laboratory branch, Division of Global Health Protection, Thailand MOPH-U.S. CDC collaboration (TUC), Nonthaburi, Thailand
2007-2017	Senior Medical Research Technologist. Strengthening Laboratory Capacity Program, Thailand MOPH-U.S. CDC collaboration (TUC), Nonthaburi, Thailand
2003-2007	Medical Research Technologist. International Emerging Infectious Program, Thailand MOPH-U.S. CDC collaboration TUC), Nonthaburi, Thailand
1999- 2003	Medical Technician. Armed Force Research Institute of Medical Sciences (AFRIMS-USAMC), Rajvithee Road, Bangkok, Thailand
1997-1999	Medical Technologist. Vejthani Hospital, Bangkok, Thailand
1995-1997	Medical Technologist. Akkachon Uttaradit Hospital, Uttaradit, Thailand

# Peptide Sequencing Based on Host-Guest Interaction-Assisted Nanopore Sensing

Hai-Chen Wu<sup>a\*</sup>

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## Abstract

Scientists have been motivated by the remarkable success of nanopore DNA sequencing to extend this technology to single-molecule protein sequencing. However, several significant obstacles must be overcome to enable the nanopore sequencing of proteins. These include the creation of a unidirectional transport system for heterogeneously charged peptide chains through a nanopore and the ability to electrically identify the 20 individual amino acids or their combinations. To address these challenges, we propose a new method for protein sequencing based on enzymatic cleavage and host-guest interaction-assisted nanopore sensing. Our research reveals that the formation of a host-guest complex between a phenylalanine-containing peptide and cucurbit[7]uril (CB[7]) allows the identities of all 20 proteinogenic amino acids to be determined by the current blockage during peptide $\subset$ CB[7] translocation through  $\alpha$ -hemolysin nanopores. Furthermore, our results demonstrate the ability to identify 19 different amino acids when an amino acid is covalently attached to a specific position on the peptide probe. We also provide a proof-of-concept demonstration of peptide sequencing by cleaving off amino acids from the C-terminus of a peptide with carboxypeptidases, then identifying the amino acids with the peptide probe in the nanopore and determining the amino acid sequence. With further optimization, this approach presents a promising new direction for nanopore-based protein sequencing.

**Short Bio:**

Hai-Chen Wu obtained his PhD in organic chemistry from University of Cambridge in 2005. He then moved to Oxford and carried out his postdoctoral research in Department of Chemistry, University of Oxford until the end of 2008. During 2009-2016, he was a principal investigator at the Key Laboratory for Biomedical Effects of Nanomaterials & Nanosafety, Institute of High Energy Physics, Chinese Academy of Sciences. Since early 2017, has been a principal investigator at the CAS Key Laboratory of Analytical Chemistry for Living Bio-systems, Institute of Chemistry, Chinese Academy of Sciences. His main research interest focuses on the development of nanopore sensors and their applications in stochastic sensing and protein sequencing studies.



# Recent Advances in Nanopore Sequencing: A Glimpse into Ten Case Studies in Thailand

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## Abstract

The advent of nanopore sequencing technology has revolutionized both DNA and RNA sequencing, fostering inclusivity in genome research by enabling a broader range of labs and educational institutions to participate actively. In the middle-income country of Thailand, the introduction of solutions from Oxford Nanopore Technologies has facilitated the establishment of cost-effective long-read sequencing facilities in numerous establishments. Situated at the Faculty of Medicine Siriraj Hospital, the Siriraj Long-Read Lab (Si-LoL) is at the forefront of harnessing this innovative technology across diverse fields of application. In this presentation, we showcase our wide-ranging collaborations with domestic and international partners, spanning academic and corporate realms. These synergistic collaborations have spurred the development and execution of a diverse array of nanopore sequencing applications throughout Thailand.

**Short Bio: Thidathip Wongsurawat, Ph.D.**

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Faculty of Medicine Siriraj Hospital, Mahidol University,  
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SCOPUS: h index = 17, Citation = 828; Publications: 75



Dr. Thidathip Wongsurawat (Tip) received her PhD from Nanyang Technological Singapore. She is currently the Group Leader of Siriraj's Long-read Lab (Si-LoL) in the Faculty of Medicine at Siriraj Hospital, Mahidol University. Tip's research interest focuses on utilizing nanopore sequencing technology combined with bioinformatics data analysis in pathogen genomics with the primary goal of translating novel ideas and approaches into clinical reality. She has trained students, researchers, and physicians to use nanopore technology to sequence the genome and transcriptome of virus, bacteria, fungi, plant, mouse, and human cell-lines, as well as the metagenome from different types of clinical samples.

**WORK EXPERIENCE:**

Oct 2022-present Head, Division of Medical Bioinformatics, Faculty of Medicine Siriraj Hospital, Thailand  
Oct 2020-present Instructor, Division of Bioinformatics and Data Management for Research,  
Mahidol University, Thailand  
Oct 2021-present Consultant, Division of Global Health Protection (DGHP), Thailand – U.S.CDC Collaboration  
(TUC)  
Nov 2022-present Consultant, Oxford Nanopore Technologies (UK)  
July 2021-present Group leader, Siriraj Long-read Lab (Si-LoL), Faculty of Medicine Siriraj Hospital  
Sept 2020-present Adjunct Faculty, Department of Biomedical Informatics, University of Arkansas for  
Medical Sciences (UAMS), USA  
2019-2020 Instructor, Department of Biomedical Informatics, UAMS, USA  
2017-2019 Post-doctoral Researcher, Biomedical Informatics, UAMS, USA  
2015-2016 Post-doctoral Researcher, Bioinformatics Institute, A\*STAR, Singapore  
2014-2015 Research Associate, Bioinformatics Institute, A\*STAR, Singapore  
2008-2009 Research Assistant, Microarray Laboratory, BIOTEC, NSTDA, Thailand  
2007-2008 Project Analyst (in Molecular Medicine), BIOTEC, NSTDA, Thailand

**EDUCATION:**

2010-2015 PhD in Computational Biology and Bioinformatics, School of Computer Engineering,  
Nanyang Technological University (NTU), Singapore  
2004-2007 MSc in Bioinformatics, School of Bioresources and Technology and School of Information  
Technology, King Mongkut's University of Technology Thonburi (KMUTT), Thailand  
2001-2004 MSc in Medical Microbiology, Chulalongkorn University (CU), Thailand  
1997-2001 BSc in Microbiology, Ubon Ratchathani University (UBU), Thailand

# Nanopore Sequencing Technology (ONT)

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## Abstract

Nanopore sequencing technology (ONT) has emerged as a pivotal tool in facilitating more accessible and affordable DNA sequencing in low-to-middle-income countries. This innovation has become vital in human genome sequencing, contributing significantly to the uncovering of extensive genetic variation in human populations. However, the analysis of data generated by this sequencing technique remains a complex process, sometimes inhibiting the full exploitation of the valuable genomic insights it offers. This presentation aims to delineate the bioinformatics strategies central to nanopore data analysis of the human genome data and variant annotation, highlighting the profound applications and advantages of this technology.

**Short Bio: Piroon Jenjaroenpun, Ph.D.**

Instructor,  
Division of Medical Bioinformatics,  
Department of Research and Development,  
Faculty of Medicine, Siriraj Hospital, Mahidol University

**Adjunct Instructor,**

University of Arkansas for Medical Sciences (UAMS), USA



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Google Scholar: <http://bit.ly/2PxUNl0>

Website: <https://www.longreadlab.com>

Google scholar: *i10*-index: 24, *h*-index: 18, Citations: 1,060

Scopus: *h*-index 14, Citations: 696

**Profile:**

Piroon Jenjaroenpun is a bioinformatician with >15 years of experience working in Next-generation sequencing (NGS) data analysis at the Bioinformatic Institute of Singapore. He pursued an MSc and Ph.D. in bioinformatics after completing his BSc in microbiology. His educational background makes him understand biological problems and allows him to discuss, suggest, and brainstorm with wet-lab scientists to solve problems. He completed his training as of postdoctoral fellow at University of Arkansas for Medical Sciences (UAMS), USA, in Third-generation sequencing data analysis, such as Pacific Biosciences and Oxford Nanopore Technology. He has published more than 30 peer-reviewed articles related to NGS. Piroon's research has been focused on developing and applying bioinformatics pipelines and tools to integrate and make sense of biological data, for example, DNA/RNA structures, microbial genomes, pathogen genomics, pathogen identification, transcriptome, metagenome, epigenome, human genomics, exome, and cancer research.



## Modification of solid-state nanopore for small nucleotide detection

Kawin Loha<sup>a</sup>, Thitikorn Boonkoom<sup>b</sup>, Ibrar Alam<sup>b</sup>, Harit Pitakjakpipop<sup>b</sup>, Poramin Boonbanjong<sup>c</sup>,  
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<sup>a</sup> School of Biomolecular Science and Engineering (BSE), Vidyasirimedhi Institute of Science and Technology (VISTEC), Rayong, Thailand.

<sup>b</sup> National Nanotechnology Center (NANOTEC), National Science and Technology Development Agency (NSTDA), Thailand Science Park, Pathum Thani, Thailand.

<sup>c</sup> Program in Translational Medicine, Faculty of Medicine Ramathibodi Hospital, Mahidol University, Bangkok, Thailand.

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### Abstract

Solid state nanopores are attractive innovative nanoscale devices, especially for single molecule sensing applications and they have been used for detecting nanoparticles or biomolecules such as protein, DNA, RNA, etc. Unlike other nucleotides, microRNA is a small non-coding molecule consisting of around 20 base pairs. MicroRNA levels involve the regulation of gene expression in the body, which have potential to be cancer biomarkers. However, detection of miRNA through bare synthetic nanopore is limited by its size, specificity, and stability, which makes it hard to distinguish the signal of translocation event from local electric noises. In fact, the average diameter of unzipped single-stranded microRNA is lower than 2 nm, and self-hybridization could occur resulting in unknown actual size and length. Thus, it is difficult and challenging to detect such target molecules without modification of target analyte to become bigger or that of nanopore surface to grab and/or interact with specific targets. Due to the great properties of synthetic materials, robustness, durability, and reusability, solid-state nanopores allow physical or chemical modification of nanopore surface to improve the sensitivity or accuracy of nanopore-based sensing toward target molecules. Therefore, in this work we aim to develop simple but effective methods for miRNA detection through modification of the inner nanopore surface. Our initial idea was to attach the complementary strand of target miRNA within the nanochannel, leading to localized hybridization in the presence of target miRNA. A self-assembled monolayer of gold-thiol interaction was employed. We designed the tail of complementary strand to have a thiol group and we modified the silicon nitride membrane by gold sputtering followed by focused ion beam etching. The success of complementary strand immobilization was evaluated before and after this process. Our final objective is to validate this modified nanopore's ability for selective miRNA detection against non-target RNAs in clinical samples.

*Keywords: solid-state nanopore, miRNA, modified nanopore, self-assembled monolayer, focused ion beam*

## Molecular uptake of antibiotics through *Sm*ChiP: Chitooligosaccharide specific channel in the pathogen *Serratia marcescens*

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### Abstract

*Serratia marcescens* (*Sm*) is a Gram-negative bacterium that poses a significant threat to immunocompromised patients due to its high infectivity and resistance to numerous antimicrobial agents. Recent research on chitin utilization in *Sm* revealed the existence of a sugar-specific porin named chitoporin (*Sm*ChiP), through which *Serratia spp.* can absorb chitin nutrients. In this study, we would like to demonstrate that chitoporin can be used as a molecular gateway for antibiotics to penetrate the bacterial cell. To assess this, susceptibility tests were conducted on *S. marcescens* ATCC®14756 and *E. coli* BL21(DE3) Omp8 Rosetta strain expressing *Sm*ChiP using the agar disc diffusion assay and Minimum Inhibitory Concentration (MIC) based on the EUCAST standardized protocol. The results demonstrated that both bacteria were sensitive to most aminoglycosides and cephalosporins antibiotics. Subsequently, we evaluated the functional role of *Sm*ChiP in the interaction with sensitive antibiotics using liposome swelling assay, fluorescence spectroscopy, and black lipid membrane (BLM) technique. Additionally, we initiated the crystallization of *Sm*ChiP in complex with sensitive antibiotics, namely ceftazidime, gentamicin and kanamycin B, under optimized conditions: D6 (Calcium chloride dihydrate, 0.1 M MES, pH 6.5, 26 % v/v PEG 350 MME) from MemGold1™, C10 (0.1 M Calcium acetate hydrate, 0.1 M MES, pH 6.0, 22 % w/v PEG 8000) from MemGold2™, and H12 (0.2 M Ammonium phosphate monobasic, 0.1 M HEPES, pH 7.0, 20 % w/v PEG 1500) from MemChanel™ screening kits. These crystals are currently undergoing x-ray diffraction to further elucidate the *Sm*ChiP-antibiotic structures. Understanding the mechanism of antibiotics uptake through *Sm*ChiP holds great promise in designing novel and effective anti-microbial drugs targeted against *Serratia marcescens*.

**Keywords:** *Serratia marcescens*, Chitoporin, Black Lipid Membrane (BLM)

# Advances in Alpha-hemolysin Preparation for Nanopore Sensing of Long Non-Coding RNA From Body Secretions

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## Abstract

Cancer is the leading cause of death worldwide. Early screening and detection can reduce cancer-related mortality and make less aggressive treatment possible. Unfortunately, current screening methods are imperfect, suffering from limited sensitivity and high rate of false-positive. There is a need for the development of a simple, portable, and highly sensitive system for cancer screening and detection. Nowadays, circulating nucleic acids (CNAs) have emerged as novel and powerful biomarkers for screening, diagnosis, prognosis, and monitoring of cancer. The overexpression of long non-coding RNA has been involved in the tumorigenesis mechanisms of many types of cancer.  $\alpha$ -hemolysin nanopore sensing offers a simple and rapid single-molecule detection technique that can directly detect circulating nucleic acids and cancer biomarkers in clinical samples, in real time, with high sensitivity and specificity. In this study, we introduce the use of biotin-labeled amino acid as a new, radioactive-free, and simple approach for  $\alpha$ -hemolysin protein preparation.  $\alpha$ -hemolysin proteins were successfully synthesized by coupling *in vitro* transcription and translation process with biotin-labeled amino acids. The activity of these  $\alpha$ -hemolysin proteins was investigated, revealing their activity to induce the lysis of red blood cells. The mean hemolytic concentrations (HU<sub>50</sub>) of  $\alpha$ -hemolysin wildtype and mutant was 28.7 and 1495.1 ng/ $\mu$ l, respectively. Our results demonstrate a novel method for  $\alpha$ -hemolysin protein preparation, which serves as the first step in the detection of long non-coding RNA using nanopore technology.

**Keywords:** Alpha-hemolysin, biotin-labeled amino acids, Nanopore, Sensor



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เพื่อให้ลูกค้าของบริษัทฯ ได้รับความพึงพอใจสูงสุด บริษัทฯ ได้มีการพัฒนาประสิทธิภาพในการให้บริการแก่ลูกค้า โดยได้มีการนำระบบ **คุณภาพมาตรฐาน ISO 9001:2015** มาใช้ในการบริหารงาน และบริษัทฯ ยังสามารถให้ **บริการสอบเทียบเครื่องมือตามมาตรฐาน ISO/IEC 17025:2005** สำหรับเครื่อง UV-VIS Spectrophotometer และเครื่อง Universal Testing Machine และจะขยายขอบเขตเพื่อให้ครอบคลุมการสอบเทียบเครื่องมือชนิดอื่นๆต่อไป

และการที่ บริษัท พาราไซแอนติฟิค จำกัด เป็นบริษัทใน **กลุ่มบริษัท พาราวิชั่น จำกัด** ซึ่งเป็นองค์กรขนาดใหญ่ชั้นนำของประเทศ ทำให้บริษัทฯ มีศักยภาพสูง สามารถให้บริการลูกค้าได้ทุกระดับ ซึ่งรวมถึงการจัดซื้อ ที่เป็นโครงการขนาดใหญ่

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## Solution of Nano for Elemental and Surface analysis

### Scanning probe microscope (SPM)

Scanning probe microscope (SPM) is an instrument used for studying surfaces at the nanoscale level. SPMs form images of surfaces using a physical probe that touches the surface of a sample to scan the surface and collect data to display image on the computer.

Application for Hard Materials : • Nanoparticles • Nanofibers  
Electronics : • Battery materials • Semiconductors • Recording media



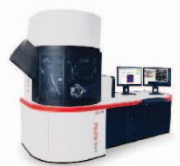
### Electron probe microanalysis (EPMA)

Electron probe microanalysis (EPMA) is used for quantitative analysis of the elemental composition of sample at a Nano - micrometer scale. The element detected by using wavelength-dispersive (WDS) spectrometers. EPMA has a broad range of applications in fields as diverse as geology, archeology, materials science, metallurgy, biology, and electronics. Battery materials • Semiconductors.

### X-ray photoelectron spectroscopy (XPS)

X-ray photoelectron spectroscopy (XPS) is a quantitative technique for measuring the elemental composition of the surface sensitive of a material can detect all elements except hydrogen and helium, and it also determines the binding states of the elements.

XPS is used to support research on surface-mediated processes such as sorption, catalysis, redox, dissolution/precipitation, corrosion, and evaporation/deposition type reactions. It is almost always the case that the surface composition and chemistry of materials, measured on the order of a few atomic layers (~3-10 nm)



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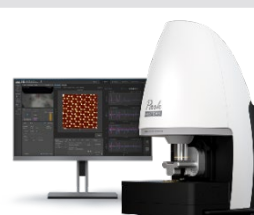
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