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Book of Abstracts

EEPM-5
2025

5th International Symposium on Energy and Environmental Photocatalytic Materials (EEPM-5)

Kuala Lumpur, Malaysia
3 – 6 November 2025

5th International Symposium on Energy and Environmental Photocatalytic Materials

EEPM-5
2025

Kuala Lumpur, Malaysia

3 – 6 November 2025

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WELCOME SPEECH

Dear Distinguished Delegates, Colleagues, and Friends,

On behalf of the Organising Committee, it is my great pleasure to welcome you to the 5th International Symposium on Energy and Environmental Photocatalytic Materials (EEPM-5), held from 3–6 November 2025 in Kuala Lumpur, Malaysia. It is an honour to host this prestigious event and to bring together a distinguished assembly of prominent researchers, early-career researchers, academicians, and industry professionals from across the globe.

Since its inception in 2014, the EEPM symposium series has established itself as a leading international platform for advancing research and fostering collaboration in the field of photocatalysis. From the inaugural EEPM-1 and EEPM-2 in Wuhan to EEPM-3 in Kraków, and EEPM-4 in Xi'an, each edition has successfully brought together experts dedicated to advancing this vital and dynamic field.

Building on this strong tradition, EEPM-5 continues to serve as a forum for the exchange of cutting-edge research, innovative technologies, and visionary ideas. The symposium features a comprehensive program including plenary lectures, keynote addresses, oral presentations, and poster sessions, covering a broad spectrum of topics, from solar fuel generation, hydrogen production, and carbon dioxide reduction, to advanced photocatalytic materials for environmental remediation, pollutant degradation, and disinfection. Emerging frontiers in semiconductor and hybrid material design, charge carrier dynamics, computational modelling, and machine learning-driven optimisation will also be highlighted, reflecting the multidisciplinary nature of this rapidly evolving field.

We hope that the discussions and interactions throughout this symposium will stimulate new perspectives and directions in photocatalysis, while strengthening research collaborations and inspiring innovative approaches towards achieving clean energy transformation, fine chemical synthesis, and environmental sustainability. EEPM-5 is not only a venue for sharing knowledge, but also a platform for building connections and fostering enduring friendships within the global photocatalysis community.

I would like to take this opportunity to extend my sincere appreciation to the members of the Organising Committee, Advisory Committee, our generous sponsors, and all contributors whose dedication and hard work have made this symposium possible. My heartfelt thanks also go to our distinguished guests and participants for enriching this event with their expertise and enthusiasm.

Finally, I warmly welcome you to Kuala Lumpur, a vibrant city that harmoniously blends tradition with modernity. I encourage you to take some time to explore its rich cultural diversity and experience the renowned hospitality of the Malaysian people.

Warm regards,

Siang-Piao Chai
Co-Chair, EEPM-5
Monash University Malaysia

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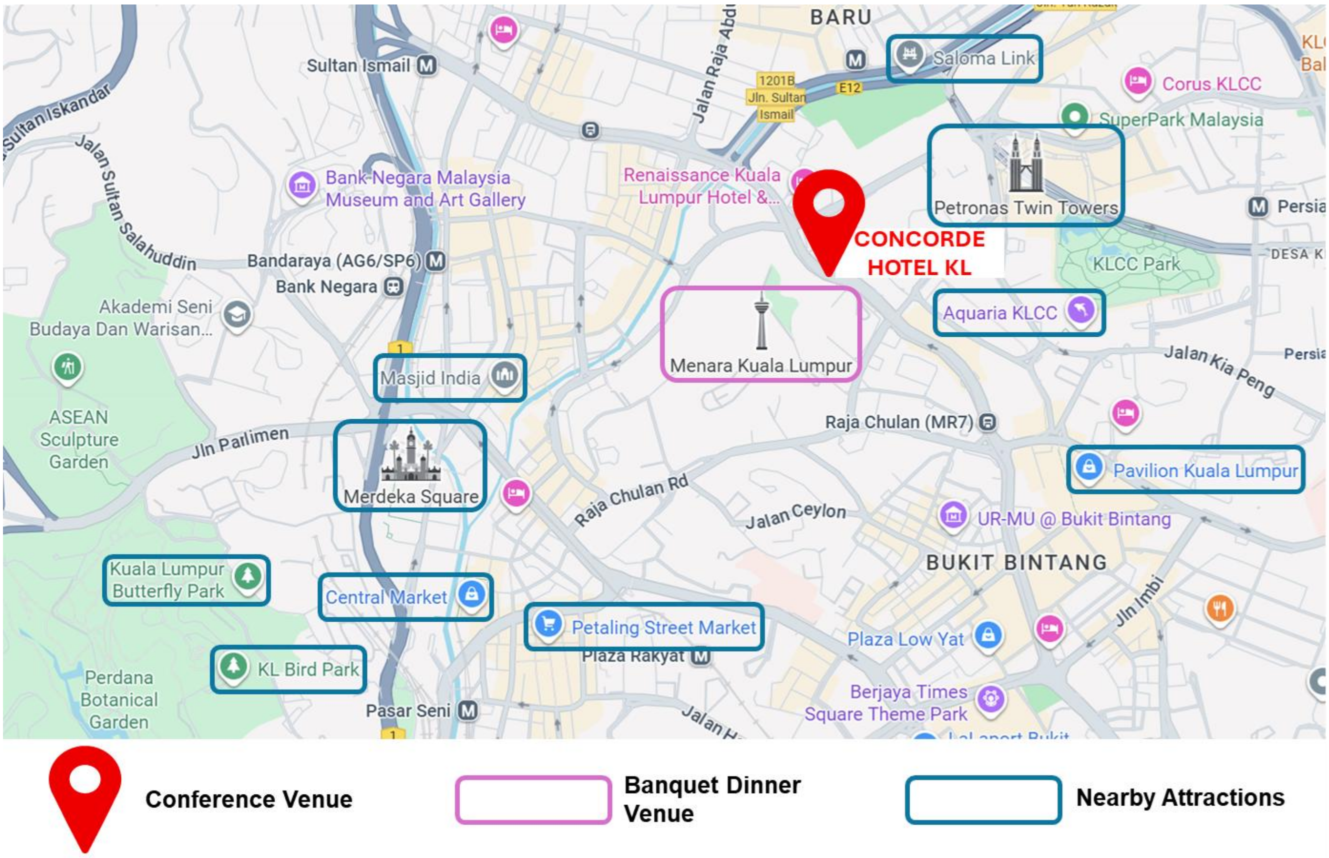
EVENT LOCATION



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CONFERENCE PROGRAM

Lecture Session

EEPM5-☐-0000

PL	**Plenary Lecture**
KL	**Keynote Lecture**
IL	**Invited Lecture**
CT	**Contributing Talk**
P	**Poster Presentation**

CONFERENCE PROGRAM

Day 1 **Monday** **3 Nov 2025**

13:00 **Registration**

18:00 **End of Day 1**

Day 2 **Tuesday** **4 Nov 2025**

08:00 **Registration**

09:00 **Opening Address, Appreciation and Photo Session**
Co-Chair: Siang-Piao Chai
Co-Chair: Jiaguo Yu

Session 1 **Session Chair: Yongfa Zhu**
09:20 [PLENARY LECTURE] EEPM5-**PL**-001
Jiaguo Yu China University of Geosciences
S-scheme Heterojunction Photocatalyst: Fundamental and Application

09:55 [KEYNOTE LECTURE] EEPM5-**KL**-004
Yun Hau Ng King Abdullah University of Science and Technology
Solar Fuels Production from Photocatalytic and Photoelectrochemical Systems

10:25 [INVITED LECTURE] EEPM5-**IL**-006
Gerko Oskam Universidad Pablo de Olavide
Charge Carrier Dynamics at Metal Oxide Photoelectrodes: Influence of Charge Extraction Kinetics

10:45 **Tea Break**

Session 2 **Session Chair: Hermenegildo Garcia**
11:05 [KEYNOTE LECTURE] EEPM5-**KL**-001
Yongfa Zhu Tsinghua University
Organic Semiconductor Photocatalysts for Water Splitting and CO_2 *Reduction under Solar Irradiation*

11:35 [INVITED LECTURE] EEPM5-**IL**-001
Chih-Wei Luo National Yang Ming Chiao Tung University
Ultrafast Dynamics of Catalytic Reaction in Quantum Materials

11:55 [INVITED LECTURE] EEPM5-**IL**-009
Zbigniew Sojka Jagiellonian University
Titania Junctions with Reduced Graphene Oxide and ZnMOF-5 Layers: A DFT+D and DFTB Investigations

12:15 [INVITED LECTURE] EEPM5-**IL**-020
Jianjun Zhang China University of Geosciences
Femtosecond Transient Absorption Spectroscopy Investigation in S-Scheme Photocatalysts

12:35 **Lunch**

Session 3 13:35	**Session Chair: Yun Hau Ng** [PLENARY LECTURE] Jimmy C Yu The Chinese University of Hong Kong *Photocatalytic Materials for a Sustainable Future*	EEPM5-**PL**-002
14:10	[KEYNOTE LECTURE] Hermenegildo Garcia Universidad Politécnica de Valencia *Metal-Organic Frameworks as Photocatalysts for Solar Fuels Production*	EEPM5-**KL**-005
14:40	[INVITED LECTURE] Xusheng Zheng University of Science and Technology of China *Application of In Situ Synchrotron Radiation Soft X-ray Resonance Spectroscopy in Photocatalysis*	EEPM5-**IL**-013
15:00	[INVITED LECTURE] Guowei Zhou Qilu University of Technology *Rational Construction of Multiporous Metal Oxide-based Photocatalysts and their Hydrogen Production Performance*	EEPM5-**IL**-018
15:20	**Tea Break**	
Session 4 15:50	**Session Chair: Zbigniew Sojka** [INVITED LECTURE] Wey Yang Teoh Universiti Malaya *Fundamental Upscaling of Photocatalytic Reactions and Complex Environment*	EEPM5-**IL**-003
16:10	[INVITED LECTURE] Wei-Kean Chong Monash University Malaysia *Water to Fuel: An Unassisted Photocatalyst System for Solar-Driven Overall Water Splitting*	EEPM5-**IL**-014
16:30	[INVITED LECTURE] Mohammad Abu Haija Khalifa University of Science and Technology *Development of Highly Efficient Ferrite-based Nanomaterials Photocatalytic Degradation of Pharmaceutical Pollutants*	EEPM5-**IL**-028
16:50	[INVITED LECTURE] Wang Wang Wuhan University of Technology *The Design and Synthesis of Catalysts for the Photosynthesis of* H_2O_2	EEPM5-**IL**-015
17:10	[INVITED LECTURE] Thanh-Binh Nguyen National Kaohsiung University of Science and Technology *Peroxymonosulfate-Assisted 0D/3D Z-Scheme* $NiCo_2O_4$*@g-*C_3N_4 *Photocatalyst with Visible-Light-Responsiveness for Effective Degradation of Ibuprofen in Water*	EEPM5-**IL**-026
17:30	**End of Day 2**	

Day 3	**Wednesday**	**5 Nov 2025**
08:00	**Registration**	
Session 5 09:00	**Session Chair: Jiaguo Yu** [PLENARY LECTURE] Hiromi Yamashita University of Osaka *Design of Nanostructured Photocatalysts for Sustainable Energy and Environmental Uses*	EEPM5-**PL**-003
09:35	[KEYNOTE LECTURE] Shaowen Cao Wuhan University of Technology *Gradient Design of Nanoscale Photocatalytic Materials*	EEPM5-**KL**-007
10:05	[INVITED LECTURE] Peng Zhou Peking University Shenzhen Graduate School *Photocatalytic Production of High-Purity Solar Hydrogen Fuel*	EEPM5-**IL**-010
10:25	**Tea Break**	
Session 6 10:45	**Session Chair: Shaowen Cao** [KEYNOTE LECTURE] Jingxiang Low Tiangong University *Solar-Driven Small Molecule Conversion for Practical Applications*	EEPM5-**KL**-003
11:15	[INVITED LECTURE] Yung-Jung Hsu National Yang Ming Chiao Tung University *Synthesis of Yolk@Shell Nanocrystals for Hydrogen Production*	EEPM5-**IL**-007
11:35	[INVITED LECTURE] Boon-Junn Ng Xiamen University Malaysia *Breaking Barriers in Soft Photocatalysis: Leveraging Excitonic Effects and Photovoltage for Overall Water Splitting*	EEPM5-**IL**-004
11:55	[INVITED LECTURE] Jingzhao Cheng Wuhan University of Technology *Confining Quantum Dots within COF Cages for Coupled* CO_2 *Photoreduction and Value-added Chemical Synthesis*	EEPM5-**IL**-016
12:15	**Lunch**	
Session 7 13:15	**Session Chair: Wee-Jun Ong** [INVITED LECTURE] Wojciech Macyk Jagiellonian University *Classification of Heterojunctions in Photocatalysis: Understanding the Fate of Photogenerated Charges*	EEPM5-**IL**-002
13:35	[INVITED LECTURE] Yuanzhi Li Wuhan University of Technology *Key Role of Light in Light-Driven Photothermocatalytic* CO_2 *Reduction by Methane on Supported Nanostructured VIII Group Metals*	EEPM5-**IL**-008

13:55	[INVITED LECTURE] Kai Dai Huaibei Normal University *Chalcogenide-based S-scheme heterojunction photocatalysts*	EEPM5-**IL**-022
14:15	[INVITED LECTURE] Muhammad Humayun Prince Sultan University *Design and Fabrication of* $TiO_2/g\text{-}C_3N_4/ZnO$ *Dual Z-Scheme Heterojunction as Efficient Photocatalyst for* H_2 *Production*	EEPM5-**IL**-019
14:35	[INVITED LECTURE] Alberto Garcia-Baldovi Universitat Politecnica de Valencia *Photocatalytic Uphill Reactions with Apparent Quantum Efficiency over 10 %*	EEPM5-**IL**-021
14:55	**Poster Presentation and Tea Break**	
Session 8 15:55	**Session Chair: Wojciech Macyk** [INVITED LECTURE] Jingrun Ran The University of Adelaide *Atomic-Level Regulation on Photocatalyst for Energy-Related Reaction*	EEPM5-**IL**-017
16:15	[INVITED LECTURE] Philippe M. Heynderickx Ghent University Global Campus *Bridging Material Modifications with Kinetic Modelling for Optimal Performance in Advanced Photocatalysis*	EEPM5-**IL**-033
16:35	[INVITED LECTURE] Jing Huang Hubei Normal University *Photothermal Synergistic Modulation of Charge Transport Behavior in Small-Polaron-Type Photoanodes for Efficient Photoelectrochemical Water Splitting*	EEPM5-**IL**-025
16:55	[INVITED LECTURE] Yi-Hao Chew Okayama University *Impact of Surface Treatment on Charge Carrier Dynamics in* Bi_4NbO_8Cl *Photocatalysts Probed by Ultrafast Time-Resolved Absorption Spectroscopy*	EEPM5-**IL**-034
17:15	[INVITED LECTURE] Alireza Ranjbari Ghent University Global Campus *Integrating Kinetic Modelling and DFT Analysis to Elucidate Phenol Degradation over* TiO_2 *Photocatalysts*	EEPM5-**IL**-035
17:35	**End of Day 3**	
18:30 – 22:30	**Banquet Dinner (Orbit Revolving Dining, KL Tower)**	

Day 4	**Thursday**	**6 Nov 2025**
08:00	**Registration**	
Session 9 09:00	**Session Chair: Jingxiang Low** [KEYNOTE LECTURE] Byeong-Kyu Lee University of Ulsan *Advanced Carbon Nitride-Based Photocatalysts for Efficient Air Purification*	EEPM5-**KL**-002
09:30	[INVITED LECTURE] Xin Ying Kong Nanyang Technological University *Plastics and Biomass Wastes as Carbon Feedstocks for Photocatalytic Synthesis of Valuable Chemicals*	EEPM5-**IL**-005
09:50	[INVITED LECTURE] Xin Li South China Agricultural University *Surface/Interface Regulation of 2D COFs-based Photocatalytic Hydrogen Production Materials*	EEPM5-**IL**-023
10:10	**Tea Break**	
Session 10 10:30	**Session Chair: Byeong-Kyu Lee** [KEYNOTE LECTURE] Wee-Jun Ong Xiamen University Malaysia *Engineering Carbon Nitride- and Metal Sulfide-based Nanomaterials for Multifunctional Solar-Powered Catalytic Applications*	EEPM5-**KL**-006
11:00	[INVITED LECTURE] Muhammad Tahir United Arab Emirates University *Multifunctional $ZnCo_2O_4/Ti_3C_2/g\text{-}C_3N_4$ Heterojunction with In-Situ Grown TiO_2 Quantum dots (QDs) for Enhanced Photocatalytic CO_2 Reduction to Solar Fuels*	EEPM5-**IL**-011
11:20	[INVITED LECTURE] Boon Tong Goh University of Malaya *Optimizing Plasma-assisted Reactive Thermal Evaporation Growth of In_2O_3 and Its Nanostructured Composites for Enhancing Hydrogen Production via Water Splitting*	EEPM5-**IL**-032
11:40	[INVITED LECTURE] Nandang Mufti Universitas Negeri Malang *Photocatalytic Degradation of Green Bromocresol using TiO_2-Ag Coated Cork Ball: Structural and Morphological Analysis*	EEPM5-**IL**-027
12:00	[INVITED LECTURE] Meng Li Nanning Normal University *Ultrafast Electron Transfer in 2D/2D $g\text{-}C_3N_4/WO_3$ S-scheme Heterojunction for Boosted H_2O_2 Production*	EEPM5-**IL**-024
12:20	**Lunch**	

Session 11	**Session Chair: Muhammad Tahir**	
13:20	[INVITED LECTURE] Sai Kishore Ravi City University of Hong Kong *Artificial and Semi-Artificial Photosynthetic Hybrid Materials for Water-Energy Nexus*	EEPM5-**IL**-012
13:40	[INVITED LECTURE] Marcin Kobielusz Jagiellonian University *Facet Engineering of* $SrTiO_3$ *for Efficient Photocatalytic Reduction of Nitroaromatics*	EEPM5-**IL**-029
14:00	[INVITED LECTURE] Soumya Ranjan Mishra Ghent University Global Campus *Oxygen-Doped* $g\text{-}C_3N_4$ *Integrated with* In_2S_3 *Quantum Dots: A Tailored n–n Heterojunction Photocatalyst for Visible-Light-Driven Antibiotic Degradation*	EEPM5-**IL**-030
14:20	[INVITED LECTURE] Naveen Kumar Maharshi Dayanand University *CuS and Ag Integrated* Sb_2O_3 *Nanosheets: Formation, Charge Transfer Enhancement and Investigation for Photocatalytic Decontamination of Organic Pollutants*	EEPM5-**IL**-031
14:40	[SPONSOR TALK] Tok Hong Yuan Interscience Sdn. Bhd. *Integrated Multi-Technique XPS Approach for In-Depth Characterization of Energy and Environmental Photocatalysts*	EEPM5-**CT**-010
15:00	**Tea Break**	
Session 12	**Student Session I** **Session Chair: Wei-Kean Chong**	
15:20	[CONTRIBUTING TALK] Sijie Wan Wuhan University of Technology *Atomic-Level Interface Design Enabling Ultrafast Charge Separation and Transfer for Photocatalytic* H_2 *Evolution*	EEPM5-**CT**-001
15:33	[CONTRIBUTING TALK] Nur Syamimi Binti Mohamad Abdul Adzis Universiti Teknologi MARA *In-Situ Constructed* $Pt\text{-}Bi_2WO_6/g\text{-}C_3N_4$ *Heterojunction with Enhanced Charge Transfer for Dual Photocatalytic Applications*	EEPM5-**CT**-007
15:46	[CONTRIBUTING TALK] Ke Ming Lim Xiamen University Malaysia *Photocatalytic Upcycling of PET Plastic Waste Integrated with* H_2 *Generation Driven by Cadmium Indium Sulfide/Cobalt Oxide Catalysts*	EEPM5-**CT**-003
15:59	[CONTRIBUTING TALK] Yulu Zhang Wuhan University of Technology *Key Role of Light in Light-Promoted Photothermocatalytic Cellulose Steam Reforming to Syngas on* Ni/La^{3+}*-doped* CeO_2	EEPM5-**CT**-004

16:12	[CONTRIBUTING TALK] Jia Guo Wuhan University of Technology *Key Role of Light in Highly Efficient Photothermocatalytic Steam Cellulose Reforming on Ni-Based Catalyst*	EEPM5-**CT**-005
16:25	**Break**	
Session 13	**Student Session II** **Session Chair: Lutfi Kurnianditia Putri**	
16:35	[CONTRIBUTING TALK] Nurul Athikah Azizan Universiti Teknologi MARA *Optimizing IMS-MOF for Photo-Electrochemical Water Treatment via Band Gap Modification*	EEPM5-**CT**-008
16:48	[CONTRIBUTING TALK] Juan Carlos Expósito-Gálvez Universidad Pablo de Olavide *Deciphering Interfacial Kinetics in Nanostructured Oxide Semiconductors for Photoelectrochemical Water Oxidation Using Intensity-Modulated Photocurrent Spectroscopy*	EEPM5-**CT**-006
17:01	[CONTRIBUTING TALK] Lei Ji Wuhan University of Technology *Pivotal Role of Light in Photothermocatalytic CO_2 Reduction by Methane on Supported Nanostructured Group VIII Metals*	EEPM5-**CT**-002
17:14	[CONTRIBUTING TALK] Lasithya Samarasinghe Deakin University *$PVDF/MoS_2/Fe_2O_3/GO$ Photocatalytic Membranes for Synchronous Cross-Flow Filtration and Photocatalysis*	EEPM5-**CT**-009
17:27	**Closing and Prize Giving**	
18:00	**End of Day 4 and Program**	

EEPM-5
2025

BOOK OF ABSTRACTS & SPEAKERS' PROFILES

EEPM5-PL-001

PLENARY SPEAKER 1

S-scheme Heterojunction Photocatalyst: Fundamental and Application

Jiaguo Yu[1,*]

[1] Laboratory of Solar Fuel, Faculty of Materials Science and Chemistry, China University of Geosciences, 68 Jincheng Street, 430078, Wuhan, China
** Corresponding Author. Email address: yujiaguo93@cug.edu.cn*

KEYWORDS: S-scheme heterojunction; history; charge transfer mechanism; characterization; application

Natural photosynthesis represents the pinnacle that green chemistry aims to achieve. Photocatalysis, inspired by natural photosynthesis and dating back to 1911, has been revitalized, offering promising solutions to critical energy and environmental challenges facing humanity today. As such, it represents a significant direction in modern chemical science. However, single photocatalyst often suffer from rapid recombination of photogenerated electrons and holes, resulting in poor activity. To correct the problems and mistakes found in type-II heterojunctions and liquid-phase Z-scheme mechanism, the innovative concept of the step-scheme (S-scheme) heterojunction was proposed in 2019 and 2020. An S-scheme heterojunction is created by combining a reduction photocatalyst (RP) and an oxidation photocatalyst (OP), which have emerged as a general method to enhance charge transfer and separation, thereby significantly improving photocatalytic performance. This report will discuss the development history, charge transfer mechanism, characterization methods and applications in S-scheme heterojunctions, providing new insight into their development and key characterization methods, including in-situ irradiated X-ray photoelectron spectroscopy, femtosecond transient absorption spectroscopy, and Kelvin probe force microscopy and so on.

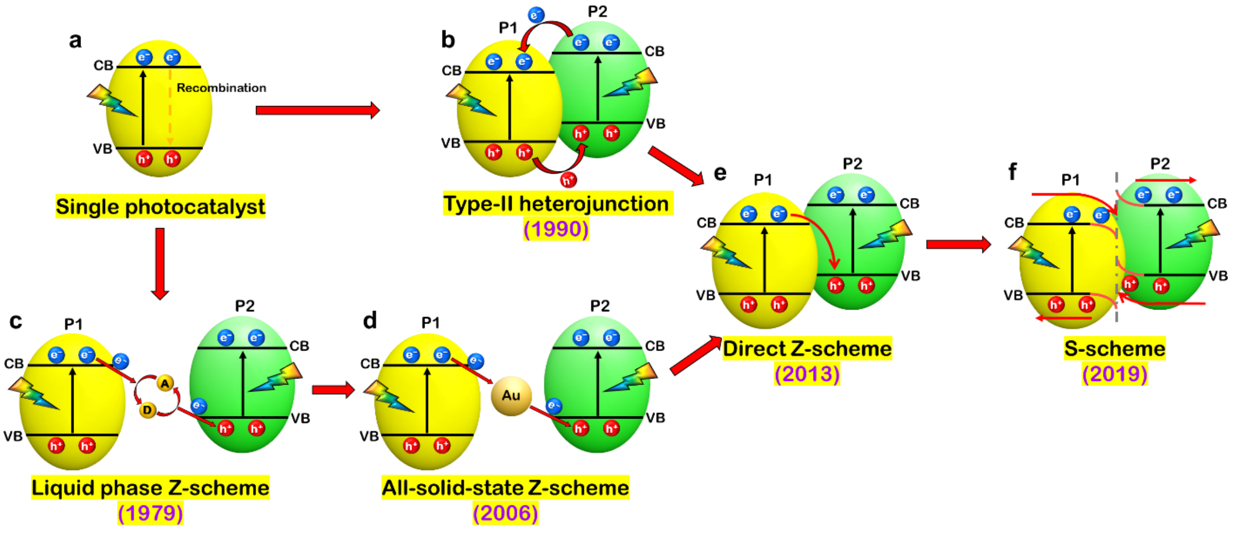

Figure 1. The development history of S-scheme heterojunction photocatalyst.

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Acknowledgements: The work was supported by the National Key Research and Development Program of China (2022YFB3803600), National Natural Science Foundation of China (22238009, U23A20102, U24A2071, 22361142704, 22261142666), and the Natural Science Foundation of Hubei Province of China (2022CFA001).

Prof. **Jiaguo Yu** is from China University of Geosciences. He received his BS and MS degrees in chemistry from Central China Normal University and Xi'an Jiaotong University, respectively, and his PhD degree in materials science in 2000 from Wuhan University of Technology. In 2000, he became a Professor at Wuhan University of Technology. In 2021, he moved to China University of Geosciences (Wuhan). His research interests include photocatalysis, adsorption, electrocatalysis, solar cells and so on. He has published more than 800 papers. He is Highly Cited Researchers in Materials Science and Chemistry since 2014. He is Foreign Member of Academia Europaea (2020), Foreign Fellow of the European Academy of Sciences (2020), Fellow of the Royal Society of Chemistry (2015), and KIA Laureate of 35th Khwarizmi International Award (khwarizmi.ir/kia/) (2022).

EEPM5-PL-002

PLENARY SPEAKER 2

Photocatalytic Materials for a Sustainable Future

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KEYWORDS: Photocatalysis; Titanium Dioxide; Carbon Nitride, Red Phosphorus

Sustainable development allows us to meet current demands without compromising the needs of future generations. Photocatalysis is a technology highly compatible with this philosophy. Many environmentally friendly materials exhibit photocatalytic functions that can be exploited for energy and environmental applications. This presentation starts with an overview of the traditional metal-based photocatalysts, [1-5] following by the development of more sustainable nonmetal photocatalytic nanomaterials. [6-10] Recent advances in strategic improvement of the efficiency and selectivity of photocatalysis systems will be examined.[11-13] Our experience in the promotion and commercialization of photocatalytic technologies will also be shared.

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Acknowledgements: The author thanks the financial support from the Research Grants Council of Hong Kong.

Prof. **Jimmy Yu** is Research Professor and Emeritus Choh-Ming Li Professor of Chemistry at The Chinese University of Hong Kong. Before retiring from teaching, he played many leadership roles including college head and department chair. Prof. Yu is a leading scientist in photocatalysis research, and he holds several patents on the fabrication and application of photocatalytic nanomaterials. He has published over 400 SCI-indexed papers with 70,000 citations (H-index: 144). Prof. Yu has received numerous honors including a State Natural Science Award and Chang Jiang Scholar Chair Professorship.

EEPM5-PL-003

PLENARY SPEAKER 3

Design of Nanostructured Photocatalysts for Sustainable Energy and Environmental Uses

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KEYWORDS: Nanostructured Photocatalysts; Porous Materials; Carbon & Hydrogen Cycling

The precise structural control of special reaction fields, such as the nanopores of zeolites, mesoporous silica, MOFs, and unique solid interfaces, was achieved. This led to the successful precise design of single-site photocatalysts (isolated metal ions, photo-functional metal complexes), ultra-fine particle semiconductor photocatalysts, plasmonic catalysts, and metal-organic framework (MOF) photocatalysts. These nano-designed high-activity photocatalysts were extended to environment-friendly reactions such as hydrogen cycling reactions (hydrogen production from water and hydrogen carrier molecules, hydrogen peroxide synthesis), carbon dioxide reduction reactions (synthesis of CO, formic acid, methanol, methane), and air-water purification, revolutionizing catalyst development.

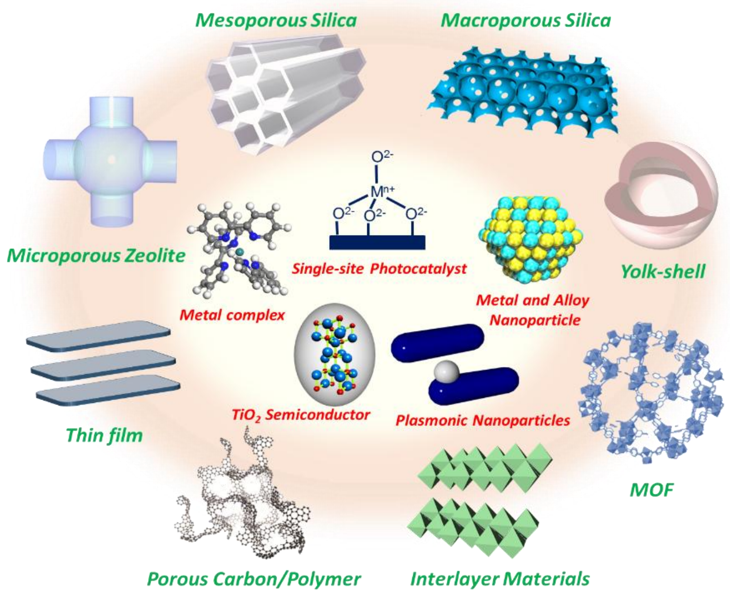

Figure 1. Design of mesostructured catalysts and photocatalysts using porous materials.

Design of Single-Site/Ultra-Fine Particle Photocatalysts in Nanospaces: The focus was made on the ability of nanoporous materials such as zeolites to fuse metal ions in an isolated state, leading to the development of "single-site photocatalysts" with structures and properties significantly different from conventional photocatalysts by introducing metal ions into pores and frameworks. Applications to CO_2 reduction and NO_X decomposition were attempted, clarifying the importance of surface coordination unsaturated sites (tetra-coordinated titanium oxide, bi-coordinate copper ions, etc.).

Furthermore, high functionality was achieved by fixing photo-functional metal complexes as single-site photocatalysts in nanospaces, applied to hydrogen production from water. On the other hand, the hybrid of ultra-fine semiconductor particles and nanoporous materials was conducted, modifying pore surfaces (with hydrocarbon, fluorine, apatite, graphene, etc.) and improving spatial characteristics (hydrophilicity/hydrophobicity, electrostatic field, spatial volume) to achieve reactant concentration and reaction efficiency. Unique higher-order nanostructures such as macro/mesoporous structures, core-shell structures, and yolk-shell (hollow space) structures were developed, leading to further activity improvements. Particularly, high-efficiency CO_2 reduction was enabled by integrating basic polymers capable of concentrating CO_2 with CO_2 reduction catalysts in hollow spaces.

Design of Plasmonic/MOF Photocatalysts Utilizing Nanostructures: Based on single-site photocatalysts, well-defined metal nanocatalysts were prepared and utilized for H_2O_2 synthesis and VOC combustion. Furthermore, by using rapid uniform heating via microwave heating and the regulated spaces of mesoporous materials, metal nanoparticles (Ag, PdAu, etc.) with precisely controlled shape, size, and color were prepared, leading to the development of plasmonic catalysts that can exhibit localized surface plasmon resonance under visible light irradiation and significantly enhance catalytic performance. Additionally, the design of metal-organic framework (MOF) photocatalysts aimed at H_2O_2 generation was conducted, creating reaction fields that inhibit the decomposition of generated H_2O_2 by hydrophobizing MOF surfaces. Furthermore, a two phases reaction system of water-organic solutions was developed, enabling the high-concentration production of H_2O_2.

Design of New Catalytic Materials Utilizing Hydrogen Spillover Phenomena: A catalyst preparation method has been developed utilizing the "hydrogen spillover phenomena," in which hydrogen molecules diffuse as atomic hydrogen on the surface of oxides through metals. Whether hydrogen diffuses on the surface of the support or is doped into the support depends on the basicity, surface functional groups, oxygen defects, and crystal phase of the oxide support. On Mo oxide, hydrogen activated by Pt spills over and is doped into the Mo oxide in large quantities, resulting in the preparation of reduced $HXMoO_{3-y}$ with numerous oxygen defects, demonstrating high activity for CO_2 reduction by functioning as a photothermal conversion catalyst under visible light irradiation. On the other hand, on oxides such as CeO_2, active hydrogen diffuses on the surface through hydrogen spillover, allowing the low-temperature rapid reduction and alloying of adjacent base metal ions. This phenomenon was utilized to develop a method for easily preparing high-entropy alloys and non-equilibrium alloy particles, designing catalysts that show high performance for CO_2 reduction, NO_X decomposition, and hydrogen production from hydrogen carrier molecules.

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Prof. **Hiromi Yamashita** has been a professor at The University of Osaka since 2004. He received PhD degree from Kyoto University in 1987. He was an assistant professor at Tohoku University, an associate professor at Osaka Prefecture University, an invited professor at University Pierre and Marie Curie (UPMC). He has been the president of Asia and Pacific Association of Catalysis Societies (APACS) (2019-2023), the president of Catalysis Society of Japan (2019-2020), the member of Academia Europea (2019-), the honorary fellow of Chinese Chemical Society (2021-), the editor of Applied Catalysis B: Environmental (2012-) and the editorial board member for several international journals. His research focuses on design of nanostructured catalysts and photocatalysts for sustainable energy and environmental uses. He has published over 650 papers (H-index: 94) and is the recipient of multiple awards from leading scientific societies including Chemical Society of Japan, Catalysis Society of Japan, Japanese Photochemistry Association, International Mesostructured Materials Association, etc. Professor Hiromi Yamashita is a professor at Osaka University and guest professor at Kyoto University, known for his research on single-site photocatalysts and nanostructured catalysts. He serves as editor of Applied Catalysis B: Environmental, and holds leadership roles in major catalysis societies in Asia.

EEPM5-KL-001

KEYNOTE SPEAKER 1

Organic Semiconductor Photocatalysts for Water Splitting and CO_2 Reduction under Solar Irradiation

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KEYWORDS: Photocatalysis; Solar Hydrogen Harvesting；CO_2 Reduction

Organic supramolecular photocatalysts with full visible spectrum response has been successfully developed. The highly crystalline perylene imide supramolecular (PDI-NH) photocatalyst is obtained with a breakthrough photocatalytic oxygen performance (40.6 mmol g^{-1} h^{-1}), which is 1353 times than the ordinary supramolecular PDI. The SA-TCPP can powerfully spilt water to hydrogen and oxygen at 40.8 and 36.1 μmol g^{-1} h^{-1} without co-catalyst. The donor-acceptor (D-A) TPPS/C_{60}-NH_2 photocatalyst was prepared by ionic self-assembly (ISA) method. The photocatalytic H_2 production rate of TPPS/C_{60}-NH_2 is greatly improved, which is 17.71 times. A highly crystalline urea-perylene imide polymer photocatalyst has been successfully built, which achieves super efficient oxygen evolution production (3223.9 μmol g^{-1} h^{-1}). Its performance is 106.5 times higher than conventional PDI supramolecular photocatalyst. The g-C_3N_4/rGO/PDIP Z-scheme heterojunction has been successfully constructed and shows an efficient and stable photocatalytic overall water splitting performance with H_2 and O_2 production rate of 15.80 and 7.80 μmol h^{-1}, respectively, about 12.1 times higher than g-C_3N_4 NS. Meanwhile, the notable AQE of 4.94% (420 nm) and solar-to-hydrogen energy conversion efficiency of 0.30% are achieved. The tetracarboxylic perylene and HOF supramolecules with hydrogen production performance of 120 mmol g^{-1} h^{-1} and 1046 mmol g^{-1} h^{-1} were obtained. In addition, an organic semiconductor photocatalyst with HOF structure was constructed by using PDI precursor, and the photocatalytic decomposition of water was realized, and the solar conversion efficiency reached 8.5%.

In addition, a photocatalyst for producing hydrogen peroxide was constructed by using organic semiconductors, and its SCC conversion efficiency could reach 2.4%. Highly selective conversion of CO_2 to ethylene, ethane, formic acid and hexose can be achieved by using MOF double copper site organic semiconductor photocatalyst.

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Prof. Dr. **Yongfa Zhu** is a full-time professor at Tsinghua University and the Deputy Director of the National Electronic Energy Spectrum Center. His research focuses on photocatalysis and its applications in environmental protection, energy conversion, and anti-tumor technologies. He serves as Editor-in-Chief of *Science for Energy and Environment*, and Associate Editor of *Green Carbon*. Furthermore, Prof. Zhu has published over 560 SCI-indexed papers, with more than 59,000 citations and an H-index of 138. He has authored five books, filed over 30 patents, and is recognized as a Highly Cited Researcher by Elsevier (since 2014) and Clarivate (since 2018). He has been supported by the Ministry of Education’s Cross-Century Excellent Talents Program and the National Natural Science Foundation of China’s Outstanding Youth Fund, and has received multiple national awards, including the Second Prize of the National Natural Science Award.

EEPM5-KL-002

KEYNOTE SPEAKER 2

Advanced Carbon Nitride-Based Photocatalysts for Efficient Air Purification

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KEYWORDS: Photocatalysis; Carbon Nitride; Air purification

Most of the world's energy still comes from fossil fuels, which release harmful gases and cause environmental problems like climate change. Photocatalysis offers a way to reduce these effects by using solar energy. Visible light-active photocatalysts, especially carbon nitride (CN), are promising due to their low cost, stability, and ability to work under natural light [1] . CN has a band gap of 2.7 eV, making it effective in applications like environmental remediation, water splitting, and CO_2 conversion. There are several methods explored for boosting photocatalytic performance, including doping, heterojunctions, vacancy engineering, and morphological control, but more sustainable and efficient methodologies are still needed [2].

Volatile organic compounds (VOCs) are the most concerning indoor air pollutants. A variety of chronic and acute health problems can be caused by long-term exposure to VOCs. Photocatalytic oxidation is a safe, efficient, and practical method for removing VOCs under mild conditions, showing strong potential for cleaner indoor air [3].

This keynote speech focuses on the green, facile, and well-engineered synthesis of CN-based photocatalysts for VOC degradation. CN-based photocatalysts were fabricated using low concentrations of WO_3 and MnO_2 metal oxides. Acetaldehyde and toluene, as well-known VOCs, were tested for photodegradation with the prepared samples. The results indicate that the cost-effective, easy-prepared, simple transition metal-based CN photocatalysts effectively remove toxic VOCs from air under solar illumination. The photodegradation performance of the CN-based photocatalysts is shown in **Figure 1a**. The density functional theory (DFT) calculation is done to show the favorable adsorption energy of acetaldehyde and toluene on the surface of the prepared photocatalysts (**Figure 1b)**. It is found that after CN modification, the adsorption energy of VOCs becomes more favorable on the surface. As a result of this modification, economic analysis indicates a reduction in electric energy consumption.

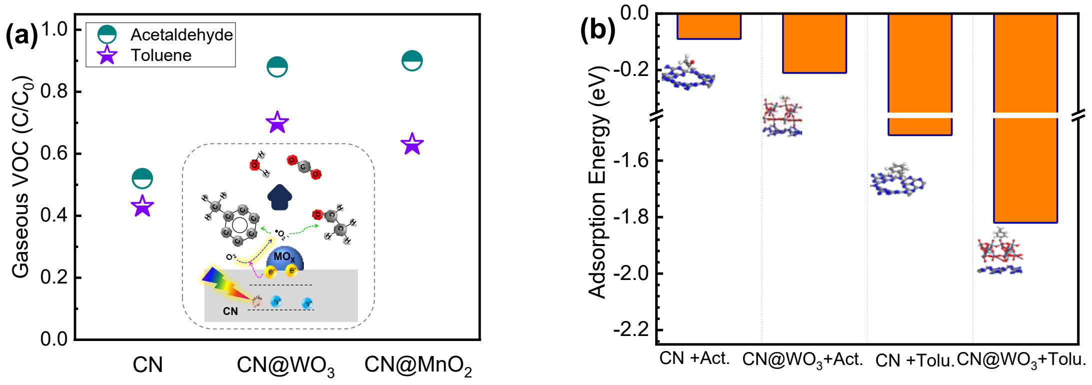

Figure 1. (a) Photodegradation of VOCs on the CN-based photocatalysts; (b) the adsorption energy of acetaldehyde and toluene on the surface of the photocatalysts.

Both experimental and theoretical analyses suggest that the enhanced photocatalytic activity results from improved light harvesting, a modified CN structure, and enhanced charge carrier separation with a lower recombination rate. The results indicate that coral-like structures effectively improve light harvesting and promote charge transfer. Metal oxides play a pivotal role in heterojunctions, redistributing electron and hole densities in photocatalysts even at trace levels.

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Acknowledgements: This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korean government (MIST) (RS-2025-00555613). ※ MSIT : Ministry of Science and ICT

Prof. **Byeong-Kyu Lee** is a Dean of Graduate School of Industry at the University of Ulsan, Korea. With a Ph.D. from University of Massachusetts (UMass) and research experience at Harvard and University of Minnesota (UMN), he is renowned for his work in photocatalysis, nanomaterials and environmental engineering. His impactful research, widely cited, focuses on sustainable technologies such as nano-zeolites, graphene, photoelectrochemical water splitting and green hydrogen production. He has published over 300 peer-reviewed papers (H-index: 65), holds 55 patents, and is the recipient of prestigious honours including Korea's Service Merit Medal and the Outstanding Professor Award from the Air & Waste Management Association (AWMA). He has been listed in the World Top 2% Scientist by Stanford/Elsevier and also listed as a Highly Ranked Scholar, Top 0.05% in Environmental Resource Management and All the fields, in ScholarGPS.

EEPM5-KL-003

KEYNOTE SPEAKER 3

Solar-Driven Small Molecule Conversion for Practical Applications

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KEYWORDS: Photocatalysis; CO_2 conversion; Ammonia production; Solar fuels; High-entropy alloys

Imitating photosynthesis in nature, photocatalytic conversion of small molecule gases (such as CO_2 and N_2) into valuable chemicals is of great significance from both the scientific and economic points of view. Amidst the development of such a technology, metal oxides have been extensively applied and studied due to their suitable band structure and excellent stability. However, the single metal oxide is confronted with low light utilization efficiency and rapid photogenerated electron-hole recombination, leading to low photocatalytic performance. To overcome these limitations, we have made a great effort in the following fields: (1) the morphology tuning of metal oxides for enhancing the light utilization of photocatalyst; (2) the loading of catalyst on metal oxides for enhancing the photogenerated charge carrier separation; (3) the design of metal oxide-based heterojunction photocatalyst for enhancing the photogenerated charge carrier utilization efficiency. The resultant systems exhibited high photocatalytic performance and improved power conversion efficiency in solar energy, which underpins important solar-energy conversion applications including solar fuel generation and environmental remediation application.

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Prof. **Jingxiang Low** is currently a Distinguished Professor at Tiangong University and serves as a principal investigator for China's National Key R&D Program and the Research Fund for International Excellent Young Scientists. He obtained his B.Eng. (Hons) from Multimedia University, Malaysia and his Master/PhD degree in materials science from Wuhan University of Technology, China. His current research interests include the developments of in situ/operando methodology toward the liquid/solid interfacial study, synthesis of metallic nanocrystals and semiconductor nanomaterials for solar energy conversion and *in situ* resource utilization. He has published more than 100 scientific papers in *Nat. Mater., Nat. Commun., J. Am. Chem. Soc., Adv. Mater., Angew. Chem. etc.*, which were cited more than 30,000 times (*h*-index: 54). He has awarded as IUPAC International Young Chemist, Clarivate Highly Cited Researcher, Elsevier Most Cited Chinese Researcher, *Nanoscale* Emerging investigator, *Chemistry of Materials* Rising Early Career Star, and CAS President's International Fellow

EEPM5-KL-004

KEYNOTE SPEAKER 4

Solar Fuels Production from Photocatalytic and Photoelectrochemical Systems

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KEYWORDS: Photocatalysis; Solar Fuels; Photoelectrochemistry

Excessive human activities have led to a series of environmental and energy issues. These issues have drawn the attention of society to seek alternatives to remediate environmental pollution and achieve a low-carbon society. Photocatalytic (PC) and photoelectrochemical (PEC) processes are considered potential ways that offer the opportunity to recycle waste, water, and carbon dioxide (CO_2), transforming them into clean hydrogen (H_2), hydrogen peroxide (H_2O_2), carbon-neutral methane (CH_4), green methanol (CH_3OH), green urea and other chemicals or fuels by using light-responsive semiconductors.

In recent years, intensive research has been devoted to exploring photoactive catalysts with ideal optoelectronic and electronic band structures that can effectively catalyze such reactions by improving light absorption, promoting charge transfer and suppressing charge carrier recombination for catalytic enhancement in PCs and PECs. Including our group, the community has made advancement and meaningful progress in understanding fundamental aspects of the catalyst development and reaction mechanisms [1-3]. However, relatively limited attention has been focused on the advanced design of photocatalytic reaction systems or reactors, which is critically vital for upscaling the overall solar energy conversion performance to an industrial scale [4].

Figure 1. Demonstration in designing scalable and integrated photocatalytic systems.

This presentation summarises our recent efforts in advancing the catalyst development, adopting engineering strategies in designing scalable and integrated light-driven catalytic systems, as illustrated in the figure above. At the end of the talk, perspectives on the challenges and outlook in constructing commercialisable PC and PEC photoreactor prototypes or devices that may become industrially viable technologies will be discussed

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Prof. **Yun Hau Ng** is an internationally recognized expert in solar energy conversion and environmental photocatalysis. He joined King Abdullah University of Science and Technology (KAUST) in 2024 as a professor of chemical engineering, where he leads the *Catalysis for Alternative & Renewable Energy (CARE)* research group. Prior to his KAUST's role, he was a faculty member at University of New South Wales (UNSW), Australia and at City University of Hong Kong. He was the Director of *Low-Carbon and Climate Impact Research Center* in Hong Kong. His research primarily focuses on developing semiconductor-based photocatalysts and photoelectrochemical systems for sunlight energy conversion, which includes hydrogen generation from water, conversion of carbon dioxide into solar fuels, and ammonia synthesis. He has received major international awards, including the *Japanese Photochemistry Association (JPA) Kataoka Award (2021)*, *APEC ASPIRE Prize (2019)* and the *Honda-Fujishima Prize (2013)*, and has secured over US$9 million in research funding from Australia and Hong Kong. Prof. Ng is also a *Clarivate Highly Cited Researcher* with more than 28,000 citations (H-index: 76) and serves as an editor for scientific journals. He currently serves as an editor for *Journal of Materials Science: Materials in Electronics (Springer);* and associate editor for *Sustainable Materials and Technologies (Elsevier)* and *Journal of Photochemistry and Photobiology A: Chemistry (Elsevier)*.

EEPM5-KL-005

KEYNOTE SPEAKER 5

Metal-Organic Frameworks as Photocatalysts for Solar Fuels Production

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KEYWORDS: Photocatalysis; Metal-Organic Frameworks; Solar Hydrogen Production; Photocatalytic CO_2 Reduction

Sunlight emitting to the Earth has an estimated power of 172 000 TW and it can provide enough energy to power the planet, whose total power required for human activities is about 20 TW, a similar power that is consumed in Natural photosynthesis. However, besides solar cells to generate electricity and some thermosolar heating applications, other uses of sunlight are still under developed and much scientific advances are needed to implement a suitable solar technology. In particular, sunlight can be used to carry out thermodynamically uphill chemical reactions that can serve to synthesize fuels, broadly denoted by Moore and Gust in the 90s as “solar fuels” [1], following the visionary concept of Ciamician in 1912. The synthesis of green and sustainable solar fuels requires of efficient photocatalysts that by absorbing photons in a wide spectral range convert them into some sort of chemical energy, such as a transient state of charge separation with the generation of electron and holes. After giving a brief overview of the possible role of solar fuels in the new sustainable, green decarbonized energy sources and the current state of the art, I will summarize the structure and properties of several of the photocatalysts studied in our group for solar fuel production from plasmonic metal oxide semiconductors to 2D nanomaterials such as transition metal sulfides and MXenes. Especial attention will be made on the photocatalytic activity of metal-organic frameworks (MOFs) and their heterojunctions with other semiconductors [2], including MOF-on-MOF, MOF supported on 2D nanomaterials such as graphene-like sheets and MXenes [3], as well as the combination of MOFs and covalent organic polymers (MOF@COFs) [4], highlighting the contributions of our group to the progress of the field [5]. Especial emphasis will be made on the structure-property relationship, the possibilities that MOFs offer to adjust the bandgap energy and the alignment of the frontiers crystal states by controlling the composition and structure of the metal nodes and by adding electron donor or withdrawing substituents on the aromatic linker. The strategy to use the available intracrystalline empty space of MOFs to host co-catalysts will be also commented, showing the contrasting activity of co-catalysts incorporated withing the pores or deposited on the external surface of the MOF crystallites. Most of the presentation will refer to the photocatalytic hydrogen generation and overall water splitting, but advances in the photocatalytic and photothermal carbon dioxide reduction and nitrogen fixation will also be briefly described. The threshold values on efficiency and photocatalyst stability to be achieved for commercial implementation of these photocatalytic processes will also be commented.

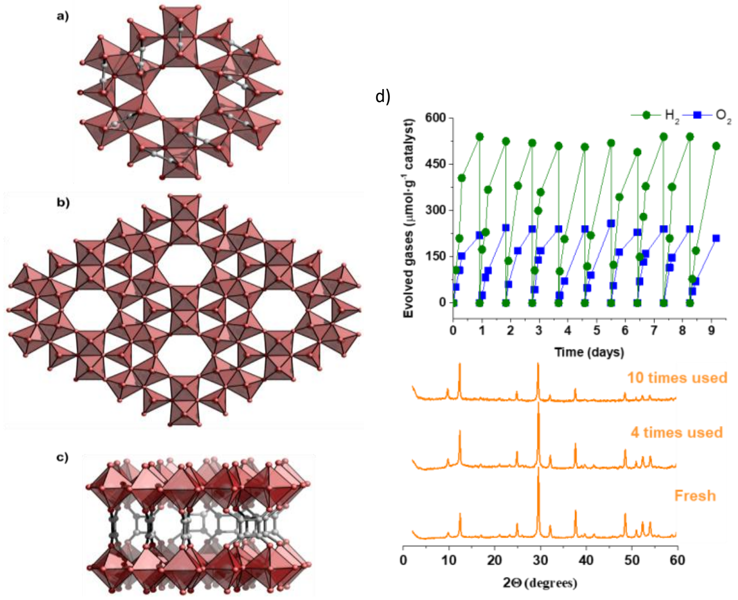

Figure 1. Structure of IEF-11 and photocatalytic H_2 and O_2 evolution upon irradiation with solar light showing IEF-11 photostability. Reproduced rom Adv. Mater., 2021 adma.202106627

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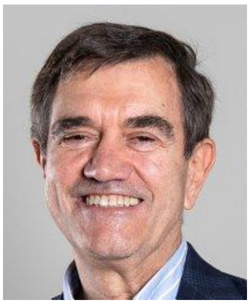
Acknowledgements: Financial support by the Spanish Ministry of Science and Innovation (CEX-2021-001230-S and PID2024-161014NB-I00 funded by MCIN/AEI/ 10.13039/501100011033), Generalitat Valenciana (CIPROM/2024/071) and Advanced Materials programme Graphica MFA/2022/023 with funding from European Union NextGenerationEU PRTR-C17.I1) and European Commission through the ERC Adv. Grant 101141466 DISCOVERY is gratefully acknowledged.



Prof. **Hermenegildo Garcia Gómez** is a distinguished professor at the Polytechnic University of Valencia (UPV) and a senior researcher at the Institute of Chemical Technology (ITQ). A globally recognized leader in photochemistry and heterogeneous catalysis, he pioneered the development of photocatalysts for solar fuel production and coined the concept of "carbocatalysis", where graphene derivatives from agricultural waste are used to convert CO_2 to methanol. With over 990 publications, 72000 citations (h-index:127) and 12 consecutive years as a Highly Cited Researcher, he was recently appointed as a full member of the Royal Academy of Exact, Physical and Natural Sciences of Spain (RAC). His numerous accolades include the Enrique Moles National Research Award (2021), the Jaume I Prize Laureate for New Technologies (2016), and the prestigious ERC Advanced Grant (2024), worth €2.5 million for development of MXene-based catalysts.

EEPM5-KL-006

KEYNOTE SPEAKER 6

Engineering Carbon Nitride- and Metal Sulfide-based Nanomaterials for Multifunctional Solar-Powered Catalytic Applications

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KEYWORDS: Carbon Nitride; Zinc Indium Sulfide; Photocatalyst; Solar-to-Chemical Conversion; Clean Energy

Among all semiconductors, carbon nitride- and transition metal sulfide-based semiconductors have emerged as promising and fascinating photocatalysts in the realm of artificial photosynthesis owing to their intrinsic properties, such as low cost, suitable band alignment, narrow band gap, etc. In recent years, the carbon nitride (i.e., C_3N_4 and C_3N_5) and ternary metal indium sulfide (e.g., $ZnIn_2S_4$, $Zn_3In_2S_6$, $Cd_2In_2S_5$, etc.) systems have been considered promising n-type semiconductors with their intrinsic properties. Despite their immense potential in solar-driven energy conversion reactions, the shortcomings of such semiconductors, including the rapid recombination of charge carriers and low oxidizing capability, hinder the photocatalytic efficiency in these applications. To overcome the encumbrances, enormous efforts from the researchers have been dedicated to the introduction of dopant, cocatalyst loading, homojunction formation, phase and morphology alteration, heterostructure construction, etc., for the realization of efficient charge separation and migration. Of note, regulating the phase and morphology of a catalyst can lead to adequate electronic band structure, active site exposure, and a shortened photocarrier migration channel. Under this backdrop, an ultrathin porous $ZnIn_2S_4$ nanosheet was prepared by our group using trisodium citrate as a shape and size controlling agent to construct a 2D nanostructure with a regular porous morphology for photocatalytic H_2 evolution and benzyl alcohol oxidation [1]. Such a porous nanosheet structure has endowed a higher surface area and an effective charge separation, resulting in an H_2 and benzaldehyde (BAD) yield of 3.98 mmol g^{-1} h^{-1} and 0.33 mmol h^{-1}, respectively. Electron paramagnetic resonance (EPR) spectroscopy and scavenger tests revealed that the photoinduced holes are the dominant reactive species to activate the cleavage of the C-H bond in benzyl alcohol to form BAD. In short, the as-prepared cocatalyst-free system effectively utilized the photogenerated charge carriers in the photoredox reaction with the aid of the nanopores and abundant active sites.

On top of that, a 2D crystalline C_3N_4 homojunction was engineered by a facile eutectic salts-assisted calcination method to enhance simultaneous H_2O_2 and benzaldehyde production without sacrificial agents [2]. The Li^+ alkaline cations stimulated PTI growth, forming the homojunction, while K^+ cations served as an electron bridge, enhancing inter-planar charge transfer and triggering cyano group (−C≡N) formation in the graphitic C_3N_4. As a result, the H_2O_2 production rate of CCN-550 reached 5838.91 μM h^{-1}, and the BAD formation rate was 7041.32 μM h^{-1}, with an AQY of 11.57 % under 420 nm light. The photoredox reaction mechanism was elucidated as a sequential two-step single-electron transfer process through the radical quenching tests, rotating disk electrode electrochemical (RRDE) analysis, and EPR. Shortly, the as-synthesized semiconductor shows that the synergistic effect of homojunction and functional group engineering can greatly accelerate charge separation and transport in carbon nitride photocatalysts. Inspired by our recent work exploring a lower C/N atomic ratio carbon nitride allotrope (C_3N_5), we have focused on synthesizing carbon-doped crystalline C_3N_5 via a liquid-phase mixing-recrystallization-polymerization strategy to precisely control the C–H functional group formation on the catalyst [3]. Such elemental doping has bestowed the improvement of HOMO–LUMO delocalization, thus enhancing charge carrier separation. The optimal sample (C-CCN$_{0.7}$) achieved 564.81 μM h^{-1} H_2O_2 and 595.37 μM h^{-1} BAD with 95% electron–hole utilization. An associative 2e$^-$ oxygen reduction reaction pathway with 70% H_2O_2 selectivity was unraveled by RRDE measurement, EPR analysis, and DFT calculation. It is worth noting that this work signifies the introduction of a targeted C–H group for tailoring the electronic structure and functional group chemistry to boost dual-functional photoredox performance.

On the other hand, the merit of heterostructure can prevail over the conflicting thermodynamic requirements for the light absorption and redox potential to enhance the transfer and lifetime of photocarriers and tailor the band structure for augmented photocatalytic properties. Notably, the electric field generated at the heterointerface, also known as the built-in electric field, is beneficial for the directional charge carrier transfer. Henceforth, it is of profound importance to pursue the mechanism for charge separation by an aptness pairing of another semiconductor with metal indium sulfides. In light of the aforementioned work, an n-type oxidative semiconductor, $W_{18}O_{49}$, coupled with $ZnIn_2S_4$ to form a Z-scheme heterojunction, leading to a remarkable production of H_2 and BAD (H_2: 122 μmol h^{-1}; BAD: 106 μmol h^{-1}) and near-unity photocarrier utilization [4]. Different from the previous case, the EPR results uncover that benzyl alcohol oxidation in Z-scheme $ZnIn_2S_4/W_{18}O_{49}$ can proceed through two different routes, which are O–H activation and C–H cleavage. By leveraging the merit of spatial charge transfer, a p-type oxidative semiconductor, Co_3O_4, can pair with $Zn_3In_2S_6$ to develop a p-n junction for ameliorating the charge recombination and redox activity by a stronger driving force [5]. The charge balance of $Zn_3In_2S_6/Co_3O_4$ is 95%, showcasing the great potential of the as-prepared system. Shortly, a photocatalyst system with a heterojunction is favorably prone to maximize the electron-hole utilization for simultaneous H_2 generation and alcohol oxidation reactions. These works endeavor to bridge the gap through the aforementioned modification strategies to facilitate the electron-hole separation process and ameliorate the charge transfer dynamics, thus enhancing the photocatalytic properties. Of note, these works can serve as a new paradigm in artificial photosynthesis for a carbon circular economy in the future.

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Prof. **Wee-Jun Ong** is the Assistant Dean and Professor in the School of Energy and Chemical Engineering (SECE) at Xiamen University Malaysia (XMUM) as well as the Director of Center of Excellence for NaNo Energy & Catalysis Technology (CONNECT). He is an Adjunct Professor at Korea University. His research focuses on photo(electro)catalytic and electrochemical H_2O splitting, CO_2 reduction, alcohol oxidation, H_2O_2 production, plastic reforming, and nitrate-to-ammonia process. He has held visiting appointments at Lawrence Berkeley National Laboratory (USA) and Technische Universität Dresden (Germany). From 2019 to 2024, he was named a Global Highly Cited Researcher (Top 1%) by Clarivate and listed among the World's Top 2% Scientists by Stanford University. With over 25,000 citations (H-index: 71), Dr. Ong is Chief Editor of *Frontiers in Nanotechnology*, Advisory Board of *Materials Horizons* and *Small*, Young Star Editor of *Nano Research* and editorial board member of several leading journals. His achievements include the Merdeka Award Grant for International Attachment and the prestigious Green Talent Award from the German Federal Ministry of Education and Research.

EEPM5-KL-007

KEYNOTE SPEAKER 7

Gradient Design of Nanoscale Photocatalytic Materials

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KEYWORDS: Charge transfer; Molecular tuning; Atomic tuning; Photocatalysis; Solar-to-chemical conversion

Excessive consumption of fossil fuels is the key contributor to climate change. Artificial photosynthetic conversion of solar energy into value-added products is considered as a promising strategy to alleviate this problem. The exploitation of low-cost, sustainable, and highly active photocatalysts is critical for improving solar-to-chemical conversion for practical applications. Hybrid photocatalytic systems have shown great potential in this field. Regulating the material structure from the atomic and molecular level to establish an ordered internal electric field that accelerates the separation of electrons and holes is vital for achieving highly efficient hybrid photocatalytic systems. Herein, we introduce the gradient design of various photocatalytic systems for target applications. (1) Donor-acceptor polymeric systems are constructed via monomer tuning, which establishes directional charge transfer channels through a built-in electric field and enhances the photocatalytic H_2O_2 production. (2) A superlattice interface and S-scheme heterojunction are carefully fabricated, building on the logical framework of universal spatial charge separation. The interfacial synergy, mediated by the internal electric field, successfully enables ultrafast spatial charge separation and transfer, resulting in highly efficient photocatalytic H_2 production. (3) Polymer/quantum dot 2D/0D systems are constructed via electrostatic adsorption–in situ growth, generating an interfacial electric field that promotes charge transfer across the interface for enhanced photocatalytic inactivation of bacteria and H_2 production.

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Prof. **Shaowen Cao** is a Professor at State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology. His current research interests include the materials development and multifunctional modulation for solar-to-chemical conversion. He is the author or co-author of more than 170 peer-reviewed scientific papers published on Nat. Commun., Chem. Soc. Rev., Adv. Mater., Angew. Chem. Int. Ed., Joule, etc., with over 25,000 citations, an H-index 72 and 22 ESI highly cited papers. He is also one of the “Highly Cited Researchers” from 2018 to 2024 awarded by Clarivate Analytics.

EEPM5-IL-001

INVITED SPEAKER 1

Ultrafast Dynamics of Catalytic Reaction in Quantum Materials

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KEYWORDS: Hydrogen Evolution Reaction; Photocatalytic CO2 Reduction; Ultrafast Dynamics

Recently, the great economic and environmental interest in producing clean fuel and chemicals through water splitting or solar-driven carbon dioxide (CO_2) reduction has been promoted worldwide, practically using 2D layered materials. In this talk, I will take the MoS_2 and $CuInP_2S_6$ as examples of the hydrogen evolution reaction (HER) and photocatalytic CO_2 reduction. Because of the ultrathin nature of 2D transition metal dichalcogenides (TMDs) catalysts, the buildup of electrolyte ions across the nanometer-scale electrochemical double layer may cause the formation of excitons and trions in monolayer (ML)-MoS_2 during HER, similar to those observed in gate-controlled FET devices [1]. Using the distinct carrier relaxation dynamics of excitons and trions as sensitive descriptors, an in-situ micro-cell-based ultrafast time-resolved liquid cell microscopy is set up to simultaneously probe the ultrafast carrier dynamics and electrochemical reactions at ML-MoS_2 catalyst during HER process [2]. It is found that the whole surface of MoS_2 becomes “trion-dominant” as the potential is at HER-on state while it becomes “exciton-dominant” as the potential is at HER-off state. Through 2D mapping image on the evolution of the individual constituents of excitons and trions on ML MoS_2 surface during HER, the interplay between exciton/trion dynamics and electrocatalytic activity of ML MoS_2 affected by electrolyte gating during HER process can be unequivocally revealed. This in-situ probing technique provides an excellent platform to explore carrier behaviors at the atomic layer/liquid electrolyte interfaces during the electrocatalytic reaction of 2D TMDs. Moreover, we also investigate the substantial influence of ferroelectric polarization on the photocatalytic CO_2 reduction efficiency, utilizing the ferroelectric-paraelectric phase transition and polarization alignment through electrical poling, and unveil its underlying mechanism by pump-probe spectroscopy [3]. These findings pave the way for manipulating electronic polarizations regulated through ferroelectric or magnetic modulations in 2D layered materials to advance the efficiency of photocatalytic CO_2 reduction.

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Acknowledgements: This work was supported by the National Science and Technology Council of the Republic of China, Taiwan with Grant: 112-2119-M-A49-012-MBK

Prof. **Chih-Wei Luo** is currently the Chairman and Professor of the Department of Electrophysics at National Yang Ming Chiao Tung University (NYCU). He leads the Ultrafast Dynamics Lab in NYCU, focusing on quantum materials, terahertz spectroscopy, and femtosecond laser research. Dr. Luo has served in key leadership roles, including Associate Vice President for International Affairs at NYCU and Chair of Taiwan’s Consortium of Emergent Crystalline Materials. He has led numerous major government-funded projects, including a Taiwan-Russia bilateral collaboration on rare-earth tellurides and advanced spectroscopy platforms. His excellence in research and teaching has earned him accolades such as the Young Scholar Outstanding Research Award and the Meritorious Teaching Award.

EEPM5-IL-002

INVITED SPEAKER 2

Classification of Heterojunctions in Photocatalysis: Understanding the Fate of Photogenerated Charges

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***KEYWORDS**: Photoinduced charge transfer, heterojunction, thermodynamics, methods in photocatalysis*

Photocatalytic systems designed for various applications often comprise two or more semiconductor components. Such composites are used to achieve an efficient charge separation, more reactive holes or electrons or other additional functionalities. However, proper classification of various heterojunctions formed of semiconductors is often difficult. We have proposed a strategy for correctly elucidating the heterojunction type [1]. It comprises three main steps: (I) the determination of band alignment, (II) the thermodynamic analysis of the interface, and (III) the verification of charge fate and charge transfer kinetics under irradiation (Figure). The experimental techniques appropriate for particular steps, including novel approaches, will be presented, together with their limitations. Following this strategy and methods of spectroscopic [2] and redox [3] characterization of semiconductors it is possible to conduct the analysis, which explores the intricate dynamics of photoinduced charges within correctly classified heterojunctions. Such a strategy gives a more reliable picture than often presented, oversimplified study.

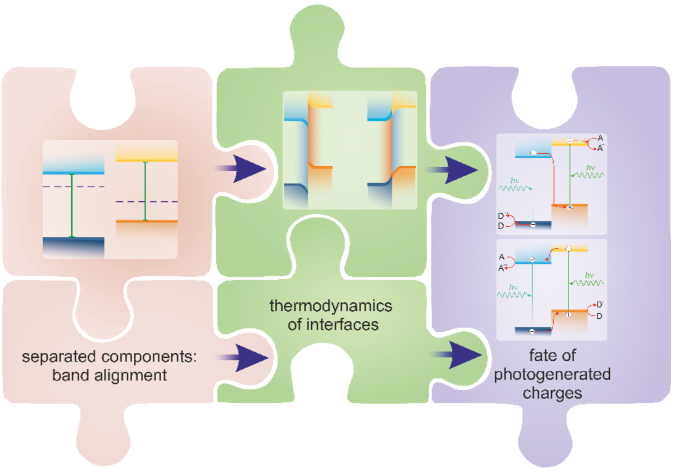

Figure 1. Determining the type of heterojunction in three consecutive steps: (I) the analysis of band alignment and Fermi levels; (II) the investigation of thermodynamic properties of the interface; (III) the verification of charge fate and charge transfer kinetics under irradiation.

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Acknowledgements: The authors acknowledge the support of the National Science Centre within the OPUS project (2022/45/B/ST5/04087).

Prof. **Wojciech Macyk** – graduated from the Jagiellonian University in Kraków (Poland), completed his PhD degree at the University of Erlangen-Nürnberg (Germany). He was the head of the Department of Inorganic Chemistry at JU (2013-2021), vice-dean (2016-2020) and the dean (2020-2024) of the Faculty of Chemistry at JU. Since 2024, he has been the vice-rector for research. In 2014 and 2015, he was a visiting professor at Hokkaido University, Sapporo, and at Western Sydney University. His research interests include mechanisms of photocatalytic processes, photocatalytic detoxification and disinfection, photocatalytic carbon dioxide fixation, photo(electro)catalytic water splitting, organic synthesis, photoelectrochemistry and spectroelectrochemistry of semiconductors. He authored >160 papers and book chapters (12,300 citations, h = 47), and several patents. Macyk is a co-founder of InPhoCat. www.photocatalysis.eu

EEPM5-IL-003

INVITED SPEAKER 3

Fundamental Upscaling of Photocatalytic Reactions and Complex Environment

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KEYWORDS: Photocatalysis; Solar Photoreactor; Photons Counting, Hydrogen

Heterogeneous photocatalysis is central to many solar-to-chemical conversions, including environmental remediation, water splitting, carbon dioxide reduction and nitrogen fixation, and as such has been attracting wide interests [1]. The efficiencies of photocatalytic reactions depend on factors that may be peculiar to other type of catalytic reactions, chief among them include light spectrum and intensity, bandgap, band potentials and photocharge dynamics [2, 3]. As such, the conventional scaling technique based on thermal-catalysed reaction often leads to failure in the implementation of photocatalysis in real environment. In this presentation, we shall revisit some fundamentals of heterogeneous photocatalysis [4]. From here, we demonstrate the basis for the unification of the two schools of thoughts, i.e., thermal- and photocatalysis, and ultimately technique for upscaling the latter. Further work shall also be presented on the prediction of photocatalytic activities in complex environment, where other non-target substrates are present such as those in wastewater [5]. The presentation shall enlighten those who are curious about upscaling photocatalytic reactions and in transferring lab data to the actual environment.

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Acknowledgements: The work is supported by the Ministry of Higher Education Malaysia via the Fundamental Research Grant Scheme (FRGS/1/2022/TK08/UM/02/43), Southeast Asia – Europe Joint Funding Scheme 2021 for Technology, Research and Innovation (HyPERMiS), and ATSE Global Science and Technology Diplomacy Fund.

Dr. **Wey Yang Teoh** is Tenured Associate Professor at the Department of Chemical Engineering, University of Malaya (UM). He gained BE and PhD in Chemical Engineering from the University of New South Wales (UNSW). Prior to UM, he was Tenured Associate Professor at the School of Energy and Environment, City University of Hong Kong, where he led the Clean Energy and Nanotechnology (CLEAN) Laboratory. His laboratory is a node of the Sunlight-to-Hydrogen Research Hub, jointly funded by the Australian Academy of Sciences (AAS) and the Academy of Technological Sciences and Engineering (ATSE). Dr Teoh's research is dedicated to the fundamentals of heterogeneous thermal- and photocatalysis, and particularly in solving various Energy and Environmentally-related problems. He currently holds Honorary Associate Professorship at UNSW, Erskine Fellowship at the University of Canterbury and serves on the Innovation Advisory Board of HeiQ AG (a leader in textile innovation). He also serves as the Chief Technology Officer of an Energy deeptech startup.

EEPM5-IL-004

INVITED SPEAKER 4

Breaking Barriers in Soft Photocatalysis: Leveraging Excitonic Effects and Photovoltage for Overall Water Splitting

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KEYWORDS: Carbon Nitride; Exciton Dissociation; Charge Asymmetry; Water Splitting

Organic carbon nitride photocatalysts have emerged as promising "soft" semiconductors for solar-driven hydrogen production. However, their overall water splitting (OWS) activity has long been constrained by tightly bound excitons and sluggish interfacial charge transfer. Herein, we demonstrate that rational excitonic modulation and charge polarization engineering can effectively overcome these intrinsic bottlenecks. Temperature-dependent photoluminescence (TDPL) measurements reveal a substantial reduction in exciton binding energy and enhanced exciton dissociation efficiency, confirming the weakened Coulomb interaction between photogenerated carriers. Furthermore, spatially resolved photo-assisted Kelvin probe force microscopy (KPFM) unveils a pronounced increase in contact potential difference under illumination, evidencing efficient migration of photoinduced charge carriers driven by a flattened interfacial barrier. These synergistic effects collectively promote charge separation and seamless electron transfer across catalytic interfaces, activating carbon nitride as a single-component light absorber for OWS in pure water. This work highlights how leveraging excitonic effects and photovoltage in soft photocatalysts can break long-standing barriers, advancing organic semiconductors toward practical solar-to-hydrogen conversion.

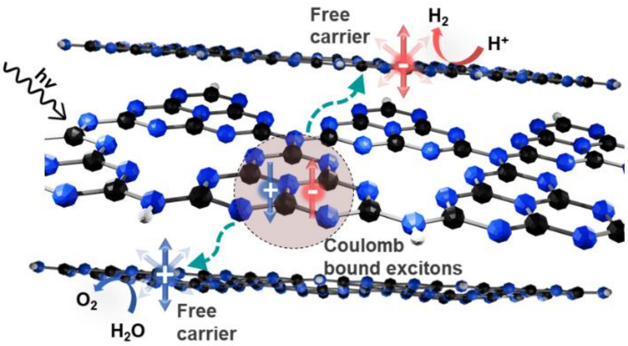

Figure 1. Schematic illustrating the working principle of organic semiconductor in photocatalysis.

Acknowledgements: The work was funded by the Ministry of Higher Education Malaysia under the Fundamental Research Grant Scheme (FRGS) (Ref. no.: FRGS/1/2023/TK05/MUSM/01/1) and Xiamen University Malaysia under Xiamen University Malaysia Research Fund (Ref. no.: XMUM/2024-C14/IENG/0071).

Dr. **Boon-Junn Ng** is an Assistant Professor at the School of Energy and Chemical Engineering, Xiamen University Malaysia. His research focuses on photocatalysis, electrocatalysis and functional nanomaterials for solar energy conversion and waste-to-value applications. He received his Ph.D. in Chemical Engineering from Monash University in 2019 and later worked as a research fellow before joining XMUM. As an early-career researcher, Dr. Ng develops advanced catalytic systems for sustainable fuel production, including water splitting for hydrogen, nitrate-to-ammonia conversion and oxidative waste transformation into value-added products.

EEPM5-IL-005 INVITED SPEAKER 5

Plastics and Biomass Wastes as Carbon Feedstocks for Photocatalytic Synthesis of Valuable Chemicals

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KEYWORDS: Plastic Upcycling; Biomass Valorization, Metal-Free Catalysts; Waste-to-Treasure Conversion

Plastic and biomass wastes represent two of the largest global waste streams and pose severe environmental concerns. The massive accumulation of these wastes not only intensifies ecological pollution, but also results in the loss of carbon resources, as both plastics and biomass are rich in carbon. In this regard, converting the embedded carbon in plastics and biomass into high-value chemicals and hydrocarbon fuels offers a promising pathway for resource recovery and waste minimization. Herein, we demonstrate a green strategy to photocatalytically upcycle a diverse range of plastics and biomass wastes into versatile chemicals at ambient conditions, in which our elegantly designed organocatalysts serve as chemical scissors to selectively cleave the inert C–C bonds in plastics and biomass to break them down into smaller, higher-value molecules.[1] Unlike conventional processes such as pyrolysis and gasification that require harsh conditions (700-1000°C) to break down these persistent plastic and biomass waste, our photocatalytic system is capable of achieving this at room temperature and atmospheric pressure. In this work, we successfully transformed a wide range of plastics, covering resin codes 1–7, as well as lignin into platform chemicals. Notably, this was accomplished without the need for pre-treatment, in contrast to many reported approaches that typically require pre-treatment of plastic and biomass in strong acidic or alkaline conditions prior to the reactions. By turning unwanted wastes into valuable chemicals, our work supports the principles of a circular economy and contributes to the pursuit of carbon neutrality.

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Dr. **Xin Ying Kong** is currently a Research Fellow at Nanyang Technological University (NTU) and holds the prestigious Lee Kuan Yew Postdoctoral Fellowship, named after the first Prime Minister of Singapore. Her research focuses on developing green and mild strategies for plastic upcycling and biomass valorization, transforming waste into hydrocarbon fuels and valuable chemicals. Recognized internationally for her contributions, she was named to the MIT Technology Review's Innovators Under 35 (TR35) Asia Pacific list in 2024 and she also received the Merdeka Award Grant in 2023.

EEPM5-IL-006

INVITED SPEAKER 6

Charge Carrier Dynamics at Metal Oxide Photoelectrodes: Influence of Charge Extraction Kinetics

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KEYWORDS: Solar water splitting; semiconductor photoelectrochemistry; intensity-modulated photocurrent spectroscopy (IMPS); electrochemical impedance spectroscopy (EIS); photocatalysis.

Photoelectrochemical water splitting is an attractive method to convert solar energy to storable chemical energy in the form of hydrogen. Metal oxide semiconductors based on abundant, low-cost materials are attractive materials related to their perceived inherent stability and sustainability for up-scaling; however, depending on the material (n-type or p-type) and cell architecture (tandem or assisted), efficiencies remain low. Hence, research has focused on the design of improvement strategies; however, it is often not clear which property or process is the main responsible for the insufficient performance.

Intensity-modulated photocurrent spectroscopy (IMPS) is a powerful technique to study the carrier dynamics: the photocurrent admittance corresponds to the frequency-dependent external quantum efficiency, and time constants for charge separation, charge transfer and surface recombination may be deduced. Based on the results, strategies can be designed to improve the performance of the system by specifically addressing the main causes of the low efficiency.

In this presentation, IMPS results on several systems representing different improvement strategies are discussed to illustrate these concepts: (i) p-$CuBi_2O_4$: competition between surface recombination and charge transfer; (ii) $WO_3/BiVO_4$ n-n junctions to improve electron extraction; (iii) thin-film $Bi_2Fe_4O_9$ with and without hole scavenger; (iv) nanostructured WO_3: effect of surface area, comparing photocatalysis and photoelectrochemistry. Key aspects that affect the interpretation of the IMPS spectra are highlighted and discussed in order to improve the understanding of efficiency-limiting processes in these complex systems. In particular, we focus on the influence that the charge extraction kinetics may have on the balance between recombination and charge transfer, thus determining the external quantum efficiency.

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Acknowledgements: The authors gratefully acknowledge funding from the Consejería de Universidad, Investigación e Innovación of the Junta de Andalucía (Spain) under grant ProyExcel_00543 (H2SOLDIR) and the Ministerio de Ciencia e Innovación of Spain, Agencia Estatal de Investigación (AEI) and EU (FEDER) under grant PID2022-140061OB-I00 (DEEPMATSOLAR). The authors also would like to thank for the support with characterization and materials analysis provided by INMALAB (Universidad Pablo de Olavide).

Prof. **Gerko Oskam** is currently a full professor of Physical Chemistry in the Department of Physical, Chemical and Natural Systems at Universidad Pablo de Olavide (UPO). His current research focuses on dye-sensitized and hybrid perovskite solar cells — emphasizing the synthesis and characterization of metal oxide nanomaterials, novel dyes, redox couples, and charge transport mechanisms — photoelectrochemical hydrogen generation using novel materials, small perturbation electrochemical methods, and solar-to-thermal energy conversion through selective coatings developed via sputtering and electrochemical deposition. He was awarded the prestigious National Chemistry Award “Andrés Manuel del Río” by the Mexican Chemical Society in 2021. Dr Oskam has published over 145 articles and several book chapters, with > 8,400 citations and a H-index of 45. His contributions continue to advance the frontiers of solar energy research and inspire innovation in sustainable energy technologies.

EEPM5-IL-007

INVITED SPEAKER 7

Synthesis of Yolk@Shell Nanocrystals for Hydrogen Production

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KEYWORDS: Yolk@Shell Nanocrystals; Hydrogen Production; Photocatalysis

This presentation emphasizes the design and synthesis of yolk@shell nanocrystals as advanced photocatalyst models. Structurally, these nanocrystals feature Au nanoparticles as the mobile inner yolk, encapsulated by an outer shell composed of hollow semiconductors. A unique aspect of yolk@shell nanocrystals is the mobility of the central Au nanoparticles, which effectively stir the reactant environment, thereby significantly accelerating catalytic processes. Moreover, the nanoreactor-like void between the yolk and shell fosters enhanced species diffusion, markedly optimizing catalytic reaction kinetics. Furthermore, the formation of a metal/semiconductor interface between the Au yolk and the semiconductor shell ensures efficient charge separation and improved photocatalytic performance. To substantiate these concepts, two exemplary yolk@shell systems developed in our laboratory, Au@Cu_7S_4 and Au@CdS, will be presented [1,2]. Both cases exemplify the versatility, efficiency, and potential applicability of yolk@shell nanocrystals, providing essential insights for the rational development of innovative photocatalysts targeting sustainable hydrogen production.

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Prof. **Yung-Jung Hsu** is a Professor of Materials Science and Engineering at National Yang Ming Chiao Tung University and serves as a Specially Appointed Professor at the Institute of Integrated Research, Institute of Science Tokyo. Having established the Nanomaterials and Optoelectronic Devices (NOD) Lab since 2007, his research group focuses on the design and characterization of semiconductor nanostructures, interfacial charge carrier dynamics, and the development of photocatalysts for renewable energy applications. He has led multiple government-funded projects, such as pioneering work on yolk@shell nanocrystals, Z-scheme photoelectrodes, and broadband light-harvesting systems for solar-driven hydrogen production. With over 140 publications (H-index: 57), Prof. Hsu also serves as an Associate Editor for ACS Applied Nano Materials (American Chemical Society) since 2024.

EEPM5-IL-008

INVITED SPEAKER 8

Key Role of Light in Light-Driven Photothermocatalytic CO_2 Reduction by Methane on Supported Nanostructured VIII Group Metals

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KEYWORDS: Photothermocatalysis; CO_2 reduction; Hydrogen production

Global warming and energy shortage owing to the combustion of fossil fuels in huge quantities are key global issues for sustainable society. Photocatalytic CO_2 reduction to produce solar fuels by using solar energy provides a very promising approach to solve the issues. However, low light-to-fuel efficiency (η) and fuel production rate (r_{fuel}) are major challenges for the photocatalytic approach. Therefore, finding a new approach of significantly increasing η and r_{fuel} is imperative and of great challenge. Recently, we developed a light-driven photothermocatalytic approach for CO_2 reduction by methane (DRM) using various catalysts of nanostructured VIII group metals supported on metal oxides such as nickel half-metal clusters supported on Al_2O_3, Co nanoparticles supported on Mg-$CoAl_2O_4$, Pd nanoparticles supported on Co and Al co-doped MgO, Ru nanoparticles supported on La modified Al_2O_3. The photothermocatalytic approach shows very high r_{fuel} and η under focused UV-vis-IR and vis-IR illumination. The approach follows a light-driven thermocatalytic DRM mechanism. It is found that the focused light not only acts as a heating role as expected, but also induces an interesting photoactivation of significantly increasing catalytic activity, which is quite different from photocatalysis on semiconductor photocatalysts. Based on a number of experimental evidences and DFT calculations, we put insight in the photoactivation for DRM on the nanostructured VIII group metal catalysts.

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Acknowledgements: The authors thank National Natural Science Foundation of China (21972109, 21673168) for awarding the grant.

Prof. **Yuanzhi Li** serves as the professor and doctoral supervisor at Wuhan University of Technology. He has led more than ten national and provincial-level research projects, including key programs under the National Key Research and Development Plan, the National Natural Science Foundation of China, and major projects of the Ministry of Education. His research focuses on photocatalysis, thermocatalysis, and photo-thermal catalysis for environmental purification and energy-related catalytic materials, where he has conducted systematic and in-depth studies. He has published over 130 SCI-indexed papers in leading international journals such as *Energy Environ. Sci., Adv. Mater., Adv. Eng. Mater., J. Am. Chem. Soc., Appl. Catal. B, Environ. Sci.Technol.* He was recognized as one of Elsevier's "Most Cited Chinese Researchers" from 2021 to 2024. His achievements have been honored with the Second Prize of the Hubei Province Natural Science Award. Furthermore, the high-efficiency non-noble metal manganese oxide VOCs purification catalysts developed by his team have been successfully industrialized and are now applied by more than 40 enterprises.

EEPM5-IL-009

INVITED SPEAKER 9

Titania Junctions with Reduced Graphene Oxide and ZnMOF-5 Layers: A DFT+D and DFTB Investigations

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KEYWORDS: Photocatalysis; tirania; graphene; MOF;DFT modelling

Fabrication of appropriate titania/organic hetero-structures plays a crucial role in the amelioration of its photo-catalytic behavior. Herein DFT/D+U and DFTB molecular modelling was applied to investigate the role of the structural and electronic properties of the ZnMOF-5|TiO_2 junction and the junction of the reduced graphene oxide (r-GO) with TiO_2 clusters of various size, ranging from small molecular Ti_2O_4 clusters into extended $Ti_{43}O_{86}$ rutile type nanocrystals of ~5 nm diameter. The electronic interactions at the r-GO|(110)TiO_2 interface give rise to net charge flow from the r-GO substrate towards the TiO_2 moieties, which was accounted for in terms of partial charge density 3D plots and formation of the interfacial dipole moments. The DOS structure of the composites was examined by means of the time dependent DFTB calculations, and the position and chemical composition of the VB and CB edges, together with the presence of mid-gap 2p C states originating from the intact graphene-like patches in the r-GO substrate were discussed in the context of conceivable photocatalytic activity of the composites. The band alignment diagram implies formation of the staggered type II scheme with the electric field offset that is sensitive to the titania cluster size. In the case of the nano-reticular TiO_2 clusters recombination of the photogenerated charges is inhibited owing to favorable spatial separation effect. For small molecular TiO_2 clusters fast cross-relaxation quenches the beneficial interfacial charge separation effect, since the strong hybridization of the oxygen and carbon states provides a convenient pathway for the efficient electronic coupling between the CB edge states of r-GO and the VB edge states of the TiO_2 moieties. A phenomenological model of molecular r-GO|Ti_2O_4 and reticular r-GO|$Ti_{43}O_{86}$ was constructed in account for different photocatalytic behavior of both junctions.

Electronic structure, bonding characteristics, adhesion and stress energy of Zn-MOF-5(100)/(110) rutile interface were modelled by periodic DFT+D method. The binding of the Zn-MOF-5 layer takes place via bidentate BDC–titania bridges. A coherent interface can be formed with the minimal periodicity along the [1-10] direction defined by nine Ti5c adsorption sites and two consecutive linkers of the Zn-MOF-5 chain. The resultant lattice strain of the Zn-MOF-5 layer is equal to $\varepsilon[001] = 0.31\ \%$ and $\varepsilon[1\text{-}10] = 2.86\ \%$, and is the associated stress energy to total = 4.8 eV. Pronounced adhesion energy of the Zn-MOF-5 layer deposited on the rutile surface (–0.33 eV/nm^2) stems from the sizable dispersion (–0.39 eV/nm^2) contribution, counterbalancing the unfavorable lattice strain and bonds distortion components. The calculated DOS structure of the Zn-MOF-5(100)/(110)TiO_2 interface shows that it can be described as an electronically coupled, staggered (Type II) charge injection system, where a photoinduced electron may be directly transferred from the Zn-MOF-5 moiety to the conduction band of the titania substrate.

Prof. **Zbigniew Sojka** is a full professor at the Department of Chemistry of the Jagiellonian University, Poland. He is an expert in experimental and computational catalysis and photocatalysis, materials and surface chemistry, spectroscopy and electron microscopy.

EEPM5-IL-010

INVITED SPEAKER 10

Photocatalytic Production of High-Purity Solar Hydrogen Fuel

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KEYWORDS: Photocatalysis, Hydrogen, Single atom, Reaction pathway

The photocatalysis technology utilizes solar energy and water directly to generate hydrogen gas, offering low cost and strong renewability [1]. Currently, the practical application of photocatalytic hydrogen production is limited by the efficiency of converting solar energy into hydrogen and the purity of produced hydrogen. Therefore, developing photocatalytic materials with high conversion efficiency and establishing a reaction pathway that enables the direct production of high-purity hydrogen have become central tasks in advancing photocatalysis for hydrogen production. In response to the above scientific challenges, this report focuses on the research of coordinating control of surface catalytic sites in the well-designed catalytic reaction pathways for the high-efficient photocatalytic production of high-purity hydrogen: (a) It explores new strategies for constructing highly reducible and thermally stable metal single-atom co-catalysts on the surface of photocatalysts (**Figure 1a**), significantly enhancing the activity and stability in hydrogen production [2-5]. (b) A photocatalytic water-reduction pathway coupled with organic reforming is developed to directly produce the high-purity hydrogen (**Figure 1b**). This strategy not only improves the hydrogen production efficiency but also enables simultaneous generation of high-purity hydrogen gas and high-value-added chemical fuels at ~100% atomic utilization efficiency [6-8].

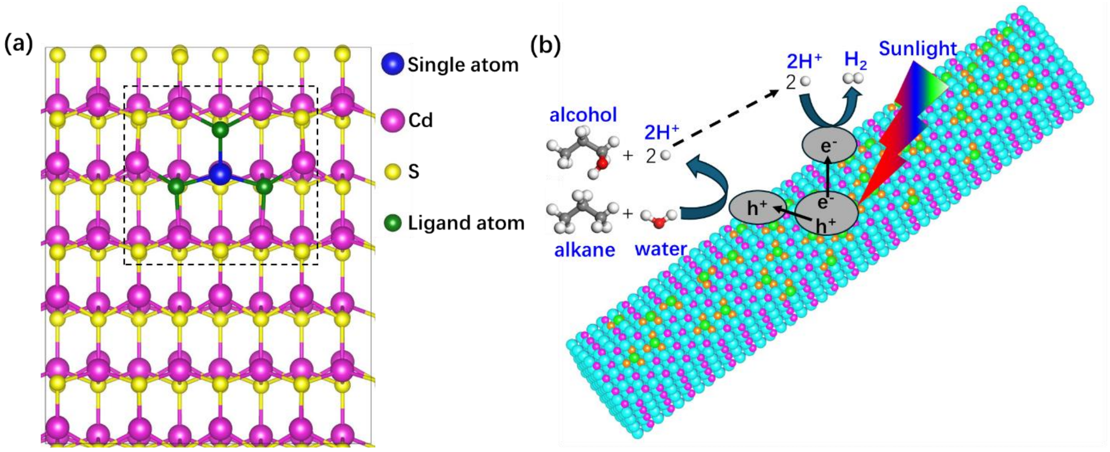

Figure 1. (a) Optimizing the coordination structure of metal single atoms in CdS photocatalyst, (b) designing the reaction pathway coupling water reduction with alkane reforming for the direct production of high-purity hydrogen and value-added organic compounds.

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Acknowledgements: The authors thank the start-up support from Peking University Shenzhen Graduate School and Shenzhen Natural Science Foundation (JCYJ20240813160123030).

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EEPM5-IL-011

INVITED SPEAKER 11

Multifunctional $ZnCo_2O_4/Ti_3C_2/g\text{-}C_3N_4$ Heterojunction with In-Situ Grown TiO_2 Quantum dots (QDs) for Enhanced Photocatalytic CO_2 Reduction to Solar Fuels

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KEYWORDS: Photocatalysis; $ZnCo_2O_4$ Nano slabs; 2D $Ti_3C_2@TiO_2$ MXenes; Solar CO_2 conversion; Green Fuels

Energy-efficient photocatalytic CO_2 conversion into sustainable solar fuels offers a promising pathway to simultaneously address both energy and environmental challenges. Selecting efficient semiconductor materials and constructing robust interfacial bonding is crucial for accelerating charge-transfer pathways and modulating reactive sites to optimize CO_2 photoreduction. Multifunctional $ZnCo_2O_4/g\text{-}C_3N_4/Ti_3C_2@TiO_2$ QDs composite with 2D layered structures was designed and fabricated for stimulating photocatalytic CO_2 reduction. The growth of TiO_2 quantum dots (QDs) over the 2D Ti_3C_2 MXene was promising to absorb visible light irradiation and effectively separate the charges. The 2D/2D $ZnCo_2O_4/g\text{-}C_3N_4$ Z-scheme heterojunction promotes strong interfacial interactions, while the incorporation of $Ti_3C_2@TiO_2$ QDs effectively suppresses the recombination of photogenerated charge carriers, thereby enhancing electron mobility. The composite stability was further confirmed through multiple reaction cycles of water splitting and CO_2 reduction, demonstrating stable and continuous production of CO and CH_4.

To mitigate CO_2 and achieve sustainable development goals (SDGs), it can be transformed into value-added fuels like CO and CH_4 for climate action and sustainability [1]. To achieve this, there is a strong demand for highly efficient and stable semiconductors capable of operating under solar energy for CO_2 reduction and hydrogen production applications [2]. Nanostructured $ZnCo_2O_4$ has generated a lot of interest as a p-type semiconductor due to its distinct electrical structure, earth-abundant, nontoxicity, and low-cost [3, 4]. Furthermore, due to its unique crystal structure and the synergistic effect of its dual-metal composition, $ZnCo_2O_4$ exhibits superior photoactivity with more abundant redox-active sites compared to single-metal oxides. However, there are few reports about the photocatalytic H_2 production and CO_2 reduction by $ZnCo_2O_4$. Thus, coupling of $g\text{-}C_3N_4$ with $ZnCo_2O_4$ to construct $ZnCo_2O_4/g\text{-}C_3N_4$ composite would be a promising approach to effectively separate photoinduced charges and also would be beneficial to maximise the photocatalytic efficiency of water splitting and CO_2 reduction reactions [5]. Among the various MXenes, $Ti_3C_2T_x$ has been most widely explored because of its low cost and promising photocatalytic characteristics due to its proper Fermi level and excellent electron transfer properties [6]. The integration of $Ti_3C_2@TiO_2$ quantum dots with $ZnCo_2O_4$ nanosheets and $g\text{-}C_3N_4$ for efficient photocatalytic CO_2 reduction, highlighting the novelty and potential impact of this approach. Therefore, constructing a $ZnCoO_4/Ti_3C_2/g\text{-}C_3N_4$ composite with a layered structure presents a promising approach. In this study, well-designed 2D $ZnCo_2O_4$ nanosheets coupled with $g\text{-}C_3N_4$ and dispersed with $Ti_3C_2@TiO_2$ QDs to form a 2D/2D/2D $g\text{-}C_3N_4/ZnCo_2O_4/Ti_3C_2@TiO_2$ QDs nanocomposite were synthesized using a hydrothermal and self-assembly approach. The photocatalytic activity of the composite under visible light irradiation was evaluated for CO_2 reduction to generate CO, CH_4, and H_2 in a continuous flow photoreactor system.

The 2D $ZnCo_2O_4$ layered structure was synthesized using a low-temperature hydrothermal synthesis method. The graphitic carbon nitride (g-C3N4) was prepared by combusting melamine in a muffle furnace at 550 °C for 2 hours. The titanium carbide (Ti_3C_2) MXene was synthesized using a room-temperature acid etching method. The HF etching process was conducted for 24 and 48 hours while continuously stirring the slurry. A simple self-assembly method was employed to synthesize various binary and ternary composites of $ZnCo_2O_4$, Ti_3C_2, and g-C_3N_4, and the final products was named as Ti_3C_2/$ZnCo_2O_4$/g-C_3N_4 (TiC-ZnC/CN) composite. Fig. 1 (a) displays the production of CO, CH_4, and H_2 during CO_2 reduction with H_2O over TiC-ZnC/CN composite. Over the entire irradiation time, CO was found to be the primary CO_2 reduction product, with smaller amounts of H_2 and CH_4. The highest CO yield of 2087 μmol g^{-1} was formed in the first cycle, which was 13.8 and 21.68 times the production of H_2 and CH_4, respectively. Furthermore, the CO production rate reached a maximum and then it was slightly decreased in the second cycle; however, the H_2 production was increased. The CO yield of 1689 μmol g^{-1} was obtained in the second cycle, which is estimated to be 7.45 and 31.94 times higher than the yield of H_2 and CH_4, respectively. In the third cyclic run, with a maximum CO yield of 1804 μmol g^{-1}, 33.62- and 89.32-times lower yields of H_2 and CH_4 were observed. The creation of CO was not linear with the irradiation period, which is more intriguing. In general, a continuous and stable amount of CO, H_2 and CH_4 was achieved in all three cycles. A proposed mechanism for the improved photocatalytic activity of the heterostructure composite is schematically illustrated in Fig. 1 (b). The formation of TiO_2 QDs over the 2D layered structure of Ti_3C_2 MXene works as a catalyst to generate charges during the photocatalysis process. Furthermore, band structures of g-C_3N_4 and $ZnCo_2O_4$ provide information about the separation and transfer process of photogenerated charge carriers. A typical Z-scheme heterojunction was formed between $ZnCo_2O_4$ and g-C_3N_4 based on their band alignment. The photogenerated electrons in the CB of $ZnCo_2O_4$ can move to the VB of g-C_3N_4 when the two materials are connected to form a 2D/2D heterojunction composite.

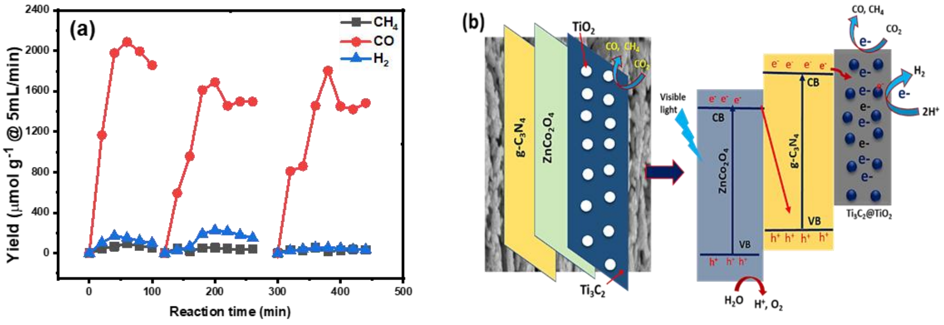

Figure 1. (a) Performance analysis of ternary composite of $ZnCo_2O_4$/Ti_3C_2/g-C_3N_4 for photocatalytic CO_2 reduction under visible light irradiation; (b) Proposed mechanism of charge separation and CO_2 reduction process under solar energy.

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Acknowledgement: This work was supported by the United Arab Emirates University (UAEU) under research grant 12R212.

Dr. **Muhammad Tahir** is an Associate Professor in the Department of Chemical and Petroleum Engineering at the United Arab Emirates University (UAEU). He has an outstanding research record with more than 310 publications in reputed international journals, serving as a single, first, and corresponding author in many of them. His work has earned him a Scopus H-index of 77 and over 16,500 citations, reflecting his strong impact in the scientific community. Dr. Tahir's research spans a wide range of areas, including photocatalysis, solar-driven water splitting and hydrogen production, solar fuel generation, and greenhouse gas CO_2 conversion. He has made significant contributions in the exploration and development of advanced materials such as MAX/MXenes, nitrides, oxides, metal–organic frameworks (MOFs) and layered double hydroxides (LDHs). Recognized globally for his scientific excellence, Dr. Tahir has received multiple national and international awards. He also contributes to the academic community as a member of the editorial boards of several high-impact journals, including *Energy and Environmental Materials*, *Energy & Fuels*, *Molecules*, and *Frontiers in Energy Research*.

EEPM5-IL-012

INVITED SPEAKER 12

Artificial and Semi-Artificial Photosynthetic Hybrid Materials for Water-Energy Nexus

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KEYWORDS: Photocatalysis; Semi-Artificial Photosynthesis, Biohybrid Materials, Solar-to-X

Can the abundantly available solar energy be tapped sustainably to meet our clean energy and clean water demands with no burden on the environment? Exploring bioinspired artificial and semi-artificial materials could hold the key. Our energy use and water use are intricately intertwined and we must of cognizant of the water footprint of energy technologies as well as the energy requirement of water technologies. Developing materials technologies for achieving sustainability in Water-Energy Nexus is therefore an important area of research. One emerging broad concept toward this goal is the idea of “Solar-to-X”. While Power-to-X is already a popular term referring to the use of electric power (ideally renewable power) for a wide range of applications like Power-to-Hydrogen, Power-to-Ammonia, Power-to-Gas, Power-to-Heat, etc. “Solar-to-X” is an emerging term that refers to a broad umbrella of technologies that capture solar energy for a wide range of applications besides electricity generation. While Solar-to-X includes both mature and niche concepts, in my talk I will touch on some of the niche concepts like Enzyme-based Solar Energy Harvesting for Bio-photovoltaics and Biocapacitors, Solar Fuels using Artificial and Semi-Artificial Photosynthetic systems, particularly from applied materials design perspective while also highlighting my past and ongoing works in these areas. The talk will focus on the structural and functional characteristics of biological photosystems that make them so attractive for green solar technologies and the work I have done to further the understanding of these photosystems in semi-artificial device setups. I will touch on the design considerations that are critical when combining biological and synthetic materials in functional devices. I will explain how aligning biotic and abiotic photophysical processes can help us design better biohybrid devices. I will conclude with an overview of challenges and open research directions in the area of artificial and semi-artificial Solar-to-X technologies.

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Acknowledgements: We thank CityUHK, Research Grants Council of Hong Kong, NUS, Ministry of Education Singapore, and National Natural Science Foundation of China for the funding support

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EEPM5-IL-013

INVITED SPEAKER 13

Application of In Situ Synchrotron Radiation Soft X-ray Resonance Spectroscopy in Photocatalysis

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KEYWORDS: Photocatalysis; Synchrotron Radiation; Resonance Spectroscopy; Soft X-ray

The global energy structure is currently undergoing a critical transition from fossil fuels to clean energy. Developing efficient and clean catalytic technologies based on renewable energy sources, such as solar energy, is of paramount importance. Utilizing solar energy to drive the conversion of inert small molecules like nitrogen (N_2), carbon dioxide (CO_2), and methane (CH_4) into fuels or high-value-added chemicals represents a crucial pathway for developing clean energy and achieving carbon neutrality. However, compared to electrocatalysis and thermal catalysis, photocatalysis still faces a significant gap in overall catalytic efficiency. As research into photocatalytic mechanisms deepens, there is an urgent need for advanced characterization techniques to unveil the intrinsic structure-activity relationships and guide the precise synthesis of high-efficiency catalysts.

Synchrotron radiation-based soft X-ray resonance spectroscopy offers inherent interface sensitivity for catalytic studies. It holds significant advantages in monitoring electron flow and dynamically evolving active sites, providing direct evidence for understanding the microscopic mechanisms of solar energy conversion, thus serving as a powerful characterization tool for mechanistic investigations. Based on this, the presenter has established a multi-spectral research platform at the photoelectron spectroscopy beamline of the Hefei Light Source (HLS), integrating techniques including in situ soft X-ray absorption spectroscopy (sXAS), resonant Auger spectroscopy (RAS), and synchrotron radiation photoelectron spectroscopy (SRPES). An in situ high-temperature/high-pressure cell with external light irradiation capability has been developed to simulate various reaction conditions, including light field, thermal field, atmosphere, and pressure. Furthermore, the presenter has utilized these developed in situ synchrotron X-ray spectroscopic techniques to probe microscopic dynamic processes within photocatalytic systems, such as photogenerated electron transfer behaviors, structural evolution of metal sites, and conversion pathways of small molecules. This work aims to identify key factors influencing photocatalytic efficiency and provide theoretical guidance for the design and optimization of novel, high-efficiency solar energy conversion materials.

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EEPM5-IL-014

INVITED SPEAKER 14

Water to Fuel: An Unassisted Photocatalyst System for Solar-Driven Overall Water Splitting

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KEYWORDS: Photocatalysis; Advanced Functional Materials; Solar Hydrogen; Water Splitting; Zinc Indium Sulfide

Hydrogen (H_2) production represents one of the most environmentally benign energy solutions, as its combustion or utilization in fuel cells generates only water as by-product with zero greenhouse gas emissions. Among various sustainable strategies, photocatalytic water splitting – driven by solar energy and photo-responsive semiconductor, stands as a compelling paradigm of eco-innovation. This process exemplifies the convergence of renewable energy utilization and environmental stewardship, leveraging suitable photocatalyst to harness sunlight for the direct decomposition of water into H_2 and oxygen (O_2). In stark contrast to conventional H_2 production methods that depend on fossil fuels, solar-driven water splitting via photocatalysis offers a carbon-neutral alternative by exploiting inexhaustible solar energy and abundant water sources.

In this work, we introduce an innovative design strategy centred on a green hollow zinc indium sulfide (gZIS) photocatalyst capable of unassisted overall water splitting under solar irradiation. The hollow hierarchical architecture of gZIS enhances exposure of active crystal facets and activates typically inert basal planes, while internal vacancies improve light absorption, facilitate charge separation, and expedite interfacial charge transfer. Systematic density functional theory (DFT) simulations reveal that vacancy-induced charge redistribution significantly lowers water activation energy barriers and accelerates surface reaction kinetics.

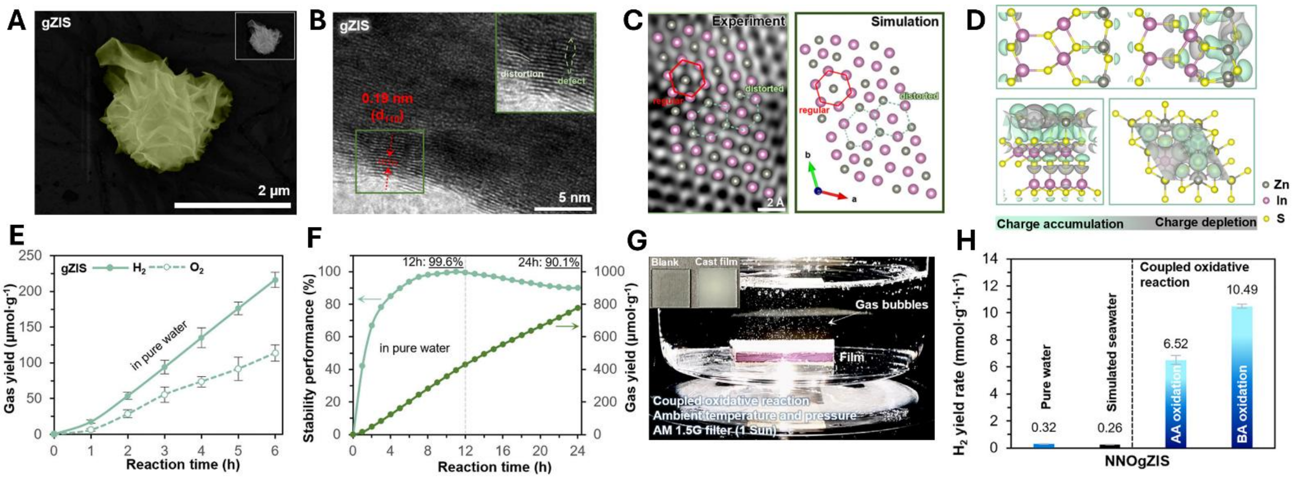

Figure 1. (A) FESEM and (B) HRTEM images illustrating the morphology of gZIS. (C-D) First-principle density functional theory on the crystal structure and charge density distribution of gZIS. (E-F) Solar-driven pure water splitting experiment on gZIS. (G-H) Practical demonstration of film-based system for modified gZIS as well as its hydrogen yield production rate under pure water, simulated seawater or with different coupled oxidation reaction.

Remarkably, the self-activated single-component gZIS achieves near-unity photostability over full-daylight operation, with a photocatalytic performance on par with other more complex sulfide-based systems. Systematic engineering and additional modification of gZIS further improves its photocatalytic water splitting activity, with broad adaptability for scalable and practical integration. These works not only demonstrate a high-efficiency photocatalyst but also establish a foundational blueprint for the rational design of next-generation materials for green hydrogen production, advancing the global pursuit of carbon neutrality.

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Acknowledgements: This research project was funded by the Malaysia Research University Network (MRUN) from the Ministry of Higher Education Malaysia (Grant No. 304/PJKIMIA/656501/K145). This work was also supported by the High Impact Research Support Fund (Ref. No. REU00354 & REU00631), High-Performance Computer (HPC) and Advanced Computing Platform (ACP) from Monash University Malaysia.

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EEPM5-IL-015

INVITED SPEAKER 15

The Design and Synthesis of Catalysts for the Photosynthesis of H_2O_2

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KEYWORDS: Photosynthesis of H_2O_2; non-sacrificial; heterojunctions; D-A conjugated polymer; $Mn_xCd_{1-x}S$; co-catalysts

The photosynthesis of hydrogen peroxide (H_2O_2) from air and water is emerging as a promising and sustainable method for producing this important chemical, which is widely used in environmental, medical, and industrial applications [1,2]. Unlike traditional anthraquinone-based processes, which are energy-intensive and environmentally taxing, photocatalytic H_2O_2 synthesis under ambient conditions offers a cleaner and potentially scalable alternative. To realize this goal, as shown in Figure 1, a series of strategies and advanced photocatalysts have been developed, including donor-acceptor (D-A) conjugated polymers and heterojunction photocatalysts, both with and without co-catalysts. These engineered materials exhibit impressive photocatalytic activity under visible light (with a H_2O_2 yield up to 6885 μmol h^{-1} g^{-1}, an AQY of 4.8% at 420 nm), achieving high selectivity and conversion efficiency. The enhanced performance of these photocatalysts (such as D-A conjugated polymers and $Mn_xCd_{1-x}S$) can be attributed to a combination of factors such as efficient charge separation, optimized energy band alignment, and favorable adsorption properties. These characteristics have been elucidated through a combination of advanced characterization techniques, such as in situ irradiated X-ray photoelectron spectroscopy (ISIXPS), and density functional theory (DFT) calculations. Together, these multifaceted insights not only reveal the underlying catalytic mechanisms responsible for the high efficiency of H_2O_2 production but also provide a theoretical and experimental foundation for the rational design of efficient photocatalysts.

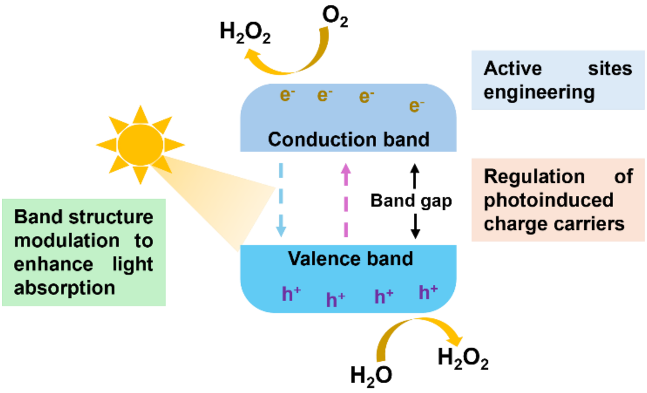

Figure 1. The strategies to enhance the efficiency of photosynthesis of H_2O_2.

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Acknowledgements: The authors thank the Hubei natural science foundation for awarding the grant (JCZRYB202500125).

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EEPM5-IL-016

INVITED SPEAKER 16

Confining Quantum Dots within COF Cages for Coupled CO$_2$ Photoreduction and Value-added Chemical Synthesis

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KEYWORDS: CO$_2$ reduction; In situ encapsulation; Porous cage; Confining effect; Microreactor

Coupling photocatalytic CO$_2$ reduction with the synthesis of value-added chemicals represents a promising strategy to mitigate carbon emissions while maximizing solar energy utilization. Quantum dots (QDs) are attractive photocatalysts for such tandem reactions, owing to their size-tunable band structures, abundant surface-active sites, and strong light-harvesting capabilities. However, their implementation is often hindered by severe aggregation and sluggish mass transfer, which limit their photocatalytic performance. Herein, we report a spatially confined 3D/0D covalent organic framework (COF)/ZnSe QDs step-scheme (S-scheme) heterojunction photocatalyst, prepared via an in-situ encapsulation strategy, for concurrent CO$_2$ photoreduction and organic transformation. The ZnSe QDs are immobilized within the nanoporous cages of the COF, forming a confined microenvironment that suppresses aggregation, enhances photostability, and promotes efficient mass transfer. As a result, the COF/ZnSe heterostructure achieves a CO generation rate of 128.3 μmol g^{-1} h^{-1}, while synchronously delivering 95.1% conversion of 1-phenylethanol to 1-phenylethanone under light irradiation. The hierarchical COF matrix acts as a nanoreactor, enriching local CO$_2$ concentration within its porous network, while the rationally designed S-scheme heterojunction facilitates directional charge flow, ensuring robust redox selectivity. This work provides a generalizable strategy for designing advanced heterostructured photocatalysts for efficient bifunctional solar chemical conversions.

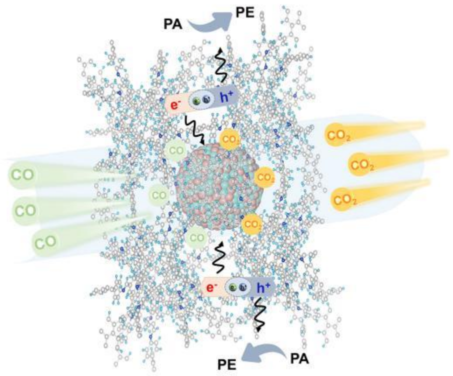

Figure 1. Illustration diagram of the working mechanism of COF/ZnSe

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Acknowledgements: This work was financially supported by the Scientific Research Innovation Capability Support Project for Young Faculty (ZYGXQNJSKYCXNLZCXM-M21), the National Natural Science Foundation of China (52472245 and 22278324), and the Natural Science Foundation of Hubei Province (2025AFA013).

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EEPM5-IL-017

INVITED SPEAKER 17

Atomic-Level Regulation on Photocatalyst for Energy-Related Reaction

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KEYWORDS: Photocatalysis; Advanced Functional Materials; Solar Hydrogen Harvesting

The global energy crisis and environmental issues impel the aggressive search for a clean and renewable energy source to replace fossil fuels. Hence, conversion of renewable solar energy into clean fuels and valuable chemicals is of great significance. The core challenge of this advanced technology lies in the development of low-cost and environmentally benign photocatalysts with sufficiently high activity and stability. Hence, the rational design and synthesis of photocatalysts at the atomic level (e.g., single-atom and dual-single-atom photocatalyst) to achieve efficient and stable solar-to-chemicals conversion is highly promising. Furthermore, both advanced characterizations (e.g., aberration-corrected atomic-resolution transmission electron microscopy, synchrotron-based X-ray absorption spectroscopy and various in-situ element/space/time-resolved characterizations) and density functional theory based theoretical computations are adopted to investigate the atomic-level structure/composition-performance relationship and mechanism in photocatalysts. The key role of these atomic-level regulation on the activity and selectivity towards H_2 evolution, CO_2 reduction, reforming plastic and reforming biomass are exhibited. Finally, a universal rule to develop high-performance photocatalysts for efficient solar-to-chemicals energy conversion is concluded.

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Acknowledgements: This work was supported by the Australian Research Council (ARC) through the Discovery Project program (FT230100192).

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EEPM5-IL-018

INVITED SPEAKER 18

Rational Construction of Multiporous Metal Oxide-based Photocatalysts and their Hydrogen Production Performance

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KEYWORDS: Photocatalysis; Multiporous Metal Oxide; S-scheme Heterojunction; Solar Hydrogen Harvesting

Environmental pollution and resource shortage become increasingly serious as the continuous development of industrialization, which are major challenges to global sustainable development. Photocatalysis technology by utilizing solar-driven reactions is poised to emerge as a reliable strategy to relieve the energy crisis and environmental pollution [1, 2]. However, the inadequate light-harvesting ability, rapid photogenerated carrier recombination, and inferior redox capacity of the individual photocatalysts restrict their photocatalytic activity for solar energy utilization. Therefore, the development of efficient semiconductor photocatalysts is a focal point of current research efforts. By considering factors such as morphology engineering, co-catalyst modification, vacancy engineering, and heterojunction construction, the photocatalysts with superior performance can be developed [3–6]. Among them, photocatalysts with multiporous structures have attracted significant attention due to their structural advantages. Their large surface area significantly increases the contact between reactants and the catalyst, improve light capture ability, thereby accelerating the kinetics of catalytic reactions. Additionally, step-scheme (S-scheme) heterojunctions can achieve efficient carrier separation at interfaces through the driving effect of an internal electric field, thus greatly enhancing the separation efficiency of photogenerated charges. Moreover, the introduction of vacancy engineering not only regulates band structures, imparting narrow bandgap characteristics and broadening the photoresponse range but also serves as centers for capturing photogenerated electrons and holes, further promoting effective carrier separation. Herein, a series of metal oxide-based photocatalysts are constructed through rational structure design and defect engineering strategies, including dual-vacancy hollow ZnO/ZnS, multi-shell Zn_2MnO_4/CdS, hierarchical flower-like $TiO_2/ZnIn_2S_4$, and vacancy-engineered flower-like TiO_2-Ov/$Zn_{0.5}Cd_{0.5}S$ S-scheme heterojunction photocatalysts, as well as layered flower-like $Ag/Ti_3C_2/TiO_2$, mesoporous TiO_2/Ti_3C_2 nanosheet, et al (Figure 1). Their applications and mechanisms in photocatalytic water splitting for hydrogen production performance are systematically explored. As the results, the multiporous metal oxide-based photocatalysts exhibit excellent photocatalytic activity for hydrogen production. This work is anticipated to offer a valuable insight for the development of multiporous structured photocatalyst.

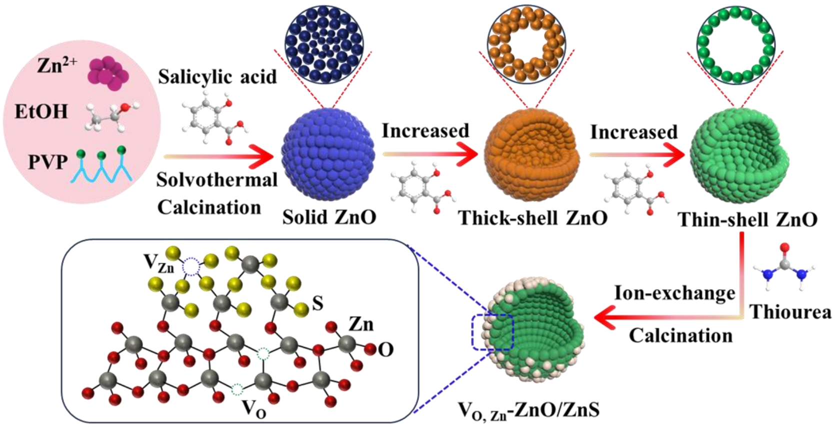

Figure 1. Schematic illustration of preparation process of hollow structured $V_{O, Zn}$-ZnO/ZnS S-scheme heterojunction.

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Acknowledgements: The authors thank the National Natural Science Foundation of China (Grant Nos. 52472215, 52202102) and Guidance Project for Interdisciplinary Innovation and Integration from Qilu University of Technology (Shandong Academy of Sciences) (Grant No. 2025XKJC0103) for awarding the grant.

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EEPM5-IL-019

INVITED SPEAKER 19

Design and Fabrication of TiO_2/g-C_3N_4/ZnO Dual Z-Scheme Heterojunction as Efficient Photocatalyst for H_2 Production

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KEYWORDS: Photocatalysis; Dual Z-scheme; Interfacial Contact; Charge Transfer; Hydrogen Production.

The development of highly effective and stable photocatalysts is crucial for green hydrogen (H_2) production through solar-driven water splitting. This study explores the design and fabrication of a TiO_2/g-C_3N_4/ZnO dual Z-scheme heterostructure photocatalyst, prepared via a wet-chemical method. The structural, morphological, and optical properties of the as-prepared heterostructure was investigated via various characterization techniques. The HRTEM image clearly indicates the formation of a ternary heterostructure, revealing distinct lattice fringes related to individual components i.e., TiO_2 (0.35 nm for the (101) plane), g-C_3N_4 (0.32 nm for the (002) plane), and ZnO (0.26 nm for the (002) plane), thereby confirming their successful integration at the nanoscale with clearly defined interfaces. The photocatalytic performance of the TiO_2/g-C_3N_4/ZnO composite was evaluated for H_2 production via water splitting. The photocatalyst revealed exceptional H_2 evolution rate (512.7 μmol h^{-1} g^{-1}) relative to the individual and binary counterparts, ascribed to the strong interfacial contact, efficient spatial separation of photoinduced charge carriers and robust redox potential. This study offers significant insights into the systematic design of multi-component Z-scheme photocatalysts for effective solar-to-hydrogen conversion.

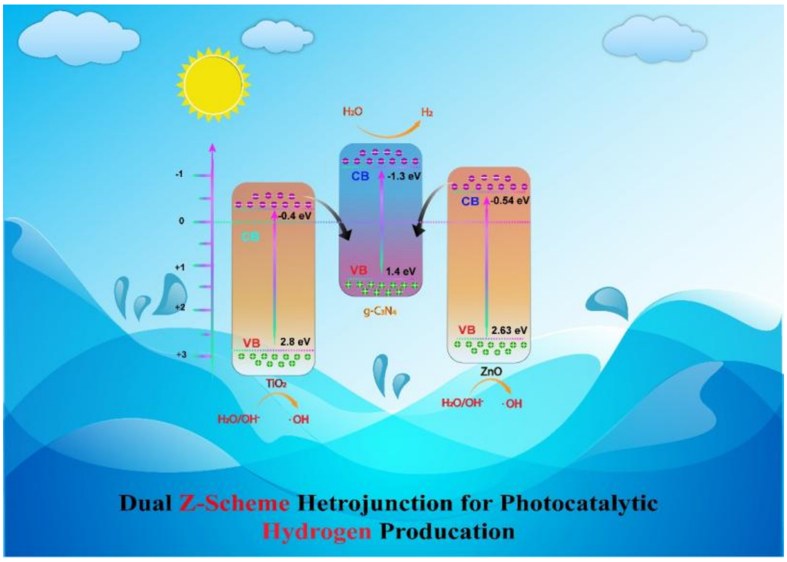

Figure 1. Schematic for band gap alignment, charge transfer and separation, and surface redox reaction over the TiO_2/g-C_3N_4/ZnO dual Z-scheme heterojunction.

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Acknowledgements: Authors would like to acknowledge Prince Sultan University, Riyadh Saudi Arabia.

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EEPM5-IL-020

INVITED SPEAKER 20

Femtosecond Transient Absorption Spectroscopy Investigation in S-Scheme Photocatalysts

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KEYWORDS: Ultrafast Spectroscopy; Fs-TAS, Electron Dynamics; S-Scheme; Interfacial Electron Transfer

The biggest challenge in the photocatalytic filed is the low photocatalytic efficiency, essentially due to the rapid recombination of photogenerated electrons and holes. In single-component photocatalyst, most photogenerated carriers are recombined inside photocatalyst (in picoseconds to nanoseconds) before migrating to the photocatalyst surface (in picoseconds) and participating in the redox reaction (in nanoseconds to microseconds). To address this issue, constructing S-scheme heterojunction photocatalysts is an effective method. S-scheme heterojunction typically consists of an oxidation semiconductor (OS) and a reduction semiconductor (RS). Under photoexcitation, the photogenerated electrons in OS conduction band will transfer to RS valence band driven by internal electric field. Consequently, photogenerated carriers with strong redox ability are spatially separated and retained in S-scheme photocatalysts. To seek the evidence of S-scheme heterojunctions, femtosecond transient absorption spectroscopy (fs-TAS) is a powerful technique that can directly monitor the ultrafast electron transfer process (in picoseconds) at RS/OS interface. Based on the fs-TAS results, the entire electron quenching dynamics of RS and OS were extracted and the lifetimes and rates of electron transfer at the RS/OS interface were obtained. In situ fs-TAS measurements with different atmospheres and solvents were also performed to simulate the actual photocatalytic process. In summary, fs-TAS can confirm the S-scheme heterojunctions from the perspective of electron transfer dynamics.

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Acknowledgements: The authors thank the National Natural Science Foundation of China (52202375), the Natural Science Foundation of Hubei Province of China (2025AFB631), and the Scientific Research Funds at China University of Geosciences (Wuhan) (Project No. 2025034).

Assoc. Prof. **Jianjun Zhang** is an Associate Professor at the Laboratory of Solar Fuel, Faculty of Materials Science and Chemistry, China University of Geosciences. His research primarily focuses on electron transfer mechanisms in photocatalysts, concentrating on utilizing femtosecond transient absorption spectroscopy to elucidate ultrafast photogenerated charge dynamics within semiconductor heterojunctions. He has led 7 projects, including grants from the National Natural Science Foundation of China and the Natural Science Foundation of Hubei Province of China. He has published over 80 papers in high-impact SCI journals such as Nat. Rev. Chem., Nat. Comm., Adv. Mater., and Angew. Chem. Int. Ed. His work has garnered over 8,800 SCI citations, with a H-index of 45. He serves as a Young Editorial Board Member for SCI journals including InfoMat, Nano-Micro Letters, and Exploration.

EEPM5-IL-021

INVITED SPEAKER 21

Photocatalytic Uphill Reactions with Apparent Quantum Efficiency over 10 %

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KEYWORDS: Photocatalysis; MOFs; Solar-to-chemicals

We propose a solar-to-chemicals photocatalysis strategy that prioritises maximising apparent quantum yield (AQY) via the simplest one-electron photochemical steps, rather than directly targeting conventional fuels (H_2 or CO_2-reduction products) [1]. Using two representative MOFs (UiO-66-NH_2 and MIL-125-NH_2) as photocatalysts [2], we demonstrate very high AQY in sacrificial, mediator-assisted schemes and argue the approach is materials-agnostic, extending to metal oxides and graphitic carbon nitrides. Analysis of band-edge positions relative to mediator redox potentials identifies energy alignment as the key bottleneck [3]; design rules around linker functionalisation, defect/metalation, and band engineering minimise overpotentials and recombination while preserving simple stoichiometry. Despite the need for sacrificial agents, this high-efficiency route can lower the threshold for economically viable photocatalytic processes and offers a tractable path to scale. Next steps include transitioning to redox-neutral pairings (eliminating sacrificial donors/acceptors), integrating tandem semi-reactions, and validating durability and photon efficiency under realistic illumination in flow.

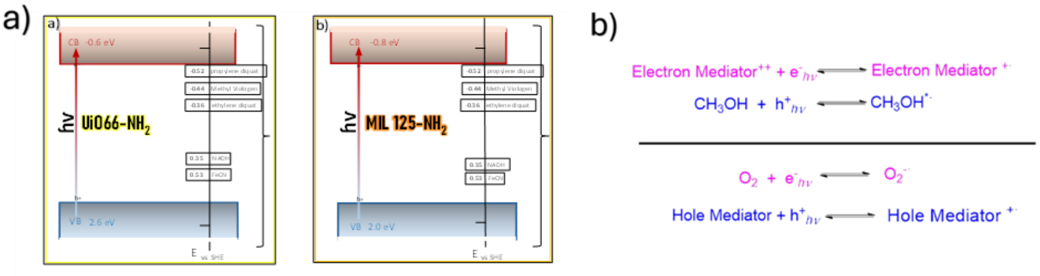

Figure 1. a) MOFs and redox mediator band gap; b) Photocatalytic reactions.

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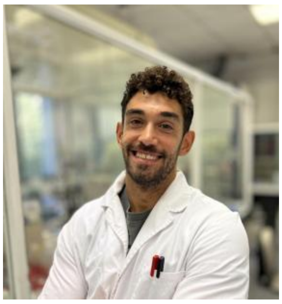
Acknowledgements: Financial support by the Spanish Ministry of Science and Innovation (CEX-2021-001230-S and PID2024-161014NB-I00 funded by MCIN/AEI/ 10.13039/501100011033) and the Generalitat Valenciana (CIPROM/2024/071 and Advanced Materials programme Graphica

MFA/2022/023 with funding from European Union NextGenerationEU PRTR-C17.I1) is gratefully acknowledged.



Alberto García Baldoví, born 9 October 1991, is a Spanish chemist and environmental scientist based in Cullera, Valencia. He earned a bachelor's degree in Chemistry from the University of Valencia, followed by a degree in Environmental Science and a master's degree at the Universitat Politècnica de València, achieving excellence in both. In 2024 he completed his PhD under Prof. Hermenegildo García Gómez at the same institution, specializing in catalysis for hydrogen generation and storage. After a postdoctoral stay at Khalifa University developing continuous-flow zeolite synthesis, he currently works at the Institute of Chemical Technology (ITQ) in Valencia on photocatalysis, CO_2 conversion, MXenes, MOFs.

EEPM5-IL-022

INVITED SPEAKER 22

Chalcogenide-based S-scheme Heterojunction Photocatalysts

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KEYWORDS: S-scheme; Photocatalysts; Chalcogenide; Charge separation

Presently, the world is confronting the dual challenges of energy scarcity and environmental pollution, with survival and development remaining paramount concerns of human society. Currently, photocatalytic water splitting for hydrogen production, photocatalytic hydrogen peroxide synthesis, and carbon dioxide reduction have emerged as highly focused and challenging areas. Emulating natural photosynthesis, utilizing long-term stable solar energy as the driving force, holds vast potential for promoting the green conversion of renewable energy and fostering sustainable development of human society. Metal chalcogenides are crucial semiconductor photocatalysts, garner significant attention due to their distinctive optical properties and electronic structures. Employing organic amines as crystal structure-directing agents, with critical implications for the morphology, structure, and properties of metal chalcogenides. It is challenging for single-component metal chalcogenide semiconductor materials to simultaneously possess a broad light absorption range and strong redox capability. The key to achieving this goal lies in constructing efficient and stable composite photocatalytic systems. Through band engineering to fabricate metal chalcogenide-based S-scheme heterojunction structure, it is anticipated to concurrently enhance light absorption efficiency, redox effect, and charge separation efficiency, thereby augmenting the photocatalytic activity of composite photocatalytic materials in water splitting for hydrogen production, hydrogen peroxide synthesis, and carbon dioxide reduction.

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Prof. **Kai Dai**: Professor of Huaibei Normal University, expert of Anhui provincial government special allowance, member of photocatalysis Committee of China photosensitive society. At present, the main research direction is semiconductor photocatalysis. He has published more than 170 SCI papers in Advanced Materials, Angewandte Chemie International Edition, Energy & Environmental Science, Advanced Functional Materials, and other international academic journals, including 17 hot paper of ESI and 40 highly cited papers of ESI. It has been cited more than 10000 times, and the h-index is 62. It has mainly undertaken more than 20 research projects above provincial and ministerial level, including NSFC, Anhui outstanding youth fund and major projects of Anhui Provincial Department of education.

EEPM5-IL-023

INVITED SPEAKER 23

Surface/Interface Regulation of 2D COFs-based Photocatalytic Hydrogen Production Materials

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KEYWORDS: Photocatalytic hydrogen production; S-scheme heterojunction; 2D COFs photocatalyst, Carrier transport separation mechanism; Exciton effects

Semiconductor photocatalysis can convert renewable solar energy into green hydrogen, which has attracted widespread attention. Recently, 2D covalent organic frameworks (COFs) with highly crystallized, adjusted and ordered structures, have proved to provide an adjustable platform for photocatalysis, especially in the field of photocatalytic hydrogen production. However, 2D COFs photocatalysts still suffer from drawbacks, such as high exciton binding energy, rapid charge carrier recombination, and insufficient active centers [1]. To address these key scientific issues, surface and interface modification of COFs semiconductors is usually required. This report introduces the recent major progress of our research group from three perspectives: local microenvironment regulation (including positional isomerization, local conjugation, heteroatom doping, and surface group modification) [2-7], precise control of active centers (including the development of ultra-thin 2D nanosheets, creation of single-molecule junctions and novel topological structures) [8-10], and S-scheme heterojunction interface regulation [11-15]. Moreover, the exciton dissociation, carrier transport separation mechanism, and photocatalytic hydrogen production mechanism of the systems were systematically studied through various methods. These studies provide reference solutions for improving the separation of charge carriers and excitons in organic photocatalysts, as well as for the promotion and application of COFs in other photocatalytic systems.

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Acknowledgements: The authors thank National Natural Science Foundation of China (22378148, 52472110, 2230082074) and Natural Science Foundation of Guangdong Province (2024A1515012433) for awarding the grant.

Prof. **Xin Li** received his BS and PhD degrees in chemical engineering from Zhengzhou University in 2002 and South China University of Technology in 2007, respectively. He joined South China Agricultural University as a faculty member, and became a professor in 2017. During 2012 and 2019, he worked as a visiting scholar at University of Texas at Austin and University of Utah, respectively. His research interests include photocatalysis, photoelectrochemistry, adsorption, biomass engineering and development of related materials and devices. As first or corresponding author, he has published 180 papers in journals such as Nature Communications, Angewandte Chemie International Edition, and Advanced Materials. He serves as board member for seven journals, including Chinese Journal of Catalysis, Acta Physico-Chimica Sinica, and Rare Metals.

EEPM5-IL-024

INVITED SPEAKER 24

Ultrafast Electron Transfer in 2D/2D g-C_3N_4/WO_3 S-scheme Heterojunction for Boosted H_2O_2 Production

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KEYWORDS: g-C_3N_4; WO_3; S-scheme heterojunction; H_2O_2 production; Oxygen reduction reaction

The escalating demand for sustainable and environmentally benign hydrogen peroxide (H_2O_2) production necessitates the development of efficient photocatalytic strategies. Herein, we report a 2D/2D g-C_3N_4/WO_3 S-scheme heterojunction synthesized via in situ growth to realize atomically intimate interface that promote ultrafast interfacial charge transfer. Extensive spectroscopic, photoelectrochemical, and density functional theory analyses unequivocally confirm the formation of a S-scheme charge transfer pathway, driven by an internal electric field that facilitates spatial separation of photogenerated charge carriers while preserving strong redox potentials. Femtosecond transient absorption spectroscopy directly reveals an ultrafast interfacial charge transfer from WO_3 to g-C_3N_4. This optimized heterostructure exhibits remarkable photocatalytic activity, achieving an H_2O_2 production rate of 2571.6 μmol g^{-1} h^{-1}, representing 2.8- and 63.5-fold improvements over g-C_3N_4 and WO_3, respectively. Electron paramagnetic resonance and in situ diffuse reflectance infrared Fourier transform spectroscopy elucidate the oxygen reduction reaction mechanism, indicating that ethanol undergoes sequential oxidation whilst photogenerated electrons reduce O_2 to produce H_2O_2. This work provides profound mechanistic insights into carrier dynamics within 2D S-scheme heterojunctions and provides a scalable and efficient route for green H_2O_2 synthesis.

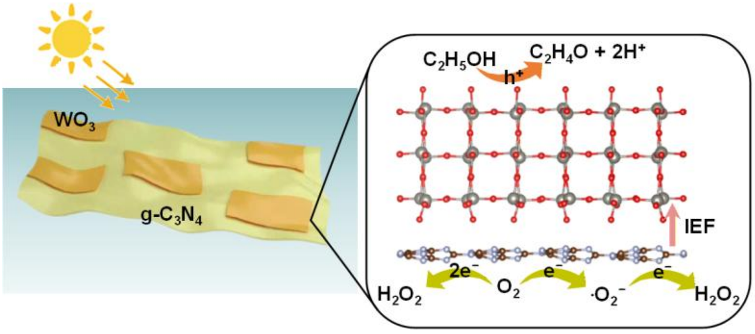

Figure 1. Schematic illustration of the working principle of g-C_3N_4/WO_3 S-scheme heterojunction.

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Acknowledgements: This work was supported by the National Natural Science Foundation of China (42207386), Natural Science Foundation of Guangxi Autonomous Region (2025GXNSFBA069543), Special Project of the Liquor Industry Research Center of Moutai Institute (MTXYJCY002).

Prof. **Meng Li** is a Master's supervisor in the School of Chemistry and Materials Science at Nanning Normal University and a visiting scholar at China University of Geosciences (Wuhan). His research centres on hydrogen peroxide production and photocatalytic degradation. He has published more than 20 SCI articles and led 4 research projects, including a National Natural Science Foundation of China Youth Program grant, a Guangxi Natural Science Foundation grant, and other funded projects.

EEPM5-IL-025

INVITED SPEAKER 25

Photothermal Synergistic Modulation of Charge Transport Behavior in Small-Polaron-Type Photoanodes for Efficient Photoelectrochemical Water Splitting

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KEYWORDS: Photoelectrochemical; Charge transport; Charge separation; Photoanodes; Water splitting

Photoelectrochemical (PEC) water splitting is a process that uses sunlight to split water for hydrogen production, holding promise for the harvesting and storing of renewable energy. Metal oxides are promising for PEC water splitting due to their excellent stability and low cost. However, their practical application faces critical limitations due to low charge separation and charge transport efficiency. This limitation originates from the small polaron hopping conduction mechanism prevalent in prototypical transition metal oxides (e.g., TiO_2, Fe_2O_3, $BiVO_4$), where carrier-induced lattice distortion severely suppresses charge mobility. To address this, our work focused on improving the separation and transport of bulk and surface charges by constructing composite photoanodes. Innovatively, a photothermal effect is also introduced to regulate the carrier transport behavior of the photoanodes by activating small polaron hopping, synergistically improving the carrier separation efficiency, injection efficiency, and transport rate. Intensity-modulated photocurrent spectroscopy analysis and density functional theory studies suggest that the relatively high temperature induced by the photothermal effect can accelerate small polaron hopping and enhance electron conductivity. Consequently, optimized photoanodes exhibit dramatically enhanced photocurrent densities, with the highest achieving a 200% improvement. The related studies provide crucial insights for the rational design of high-efficiency photoelectrodes and underpin future advances in promoting PEC and photocatalytic performances of small-polaron-type semiconductors.

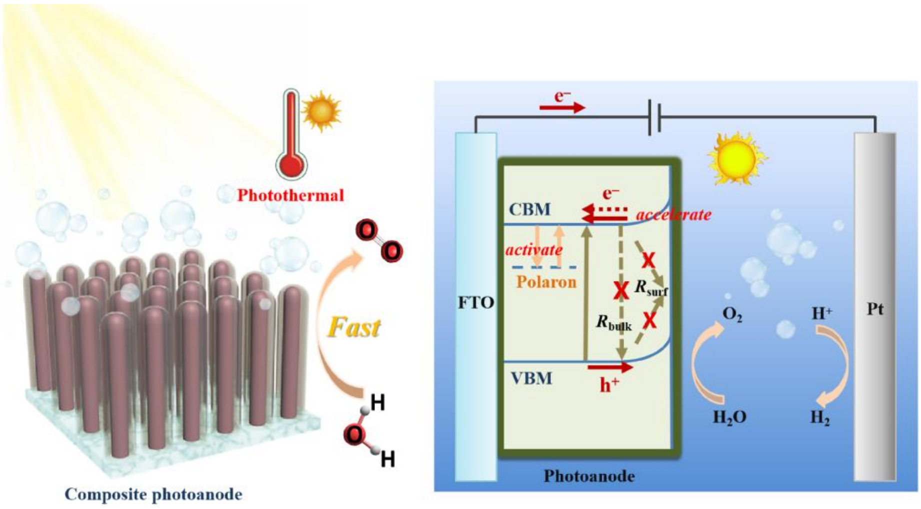

Figure 1. Mechanism schemes of the enhanced PEC performance of the small-polaron-type photoanode via the photothermal effect.

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Prof. **Jing Huang** is currently an Assistant Professor at the School of Chemistry and Chemical Engineering in Hubei Normal University. During her PhD, she received a grant from the China Scholarship Council to further her research at Nanyang Technological University. She specializes in photo(electro)catalysts and functional nanomaterials for green fuel production and solar energy conversion, with publications in reputable journals such as Carbon Energy, Nano Energy, and Chemical Engineering Journal. She also held an industry-academia-research collaboration project. She is committed to advancing the development of sustainable energy technologies through her research.

EEPM5-IL-026

INVITED SPEAKER 26

Peroxymonosulfate-Assisted 0D/3D Z-Scheme $NiCo_2O_4$@g-C_3N_4 Photocatalyst with Visible-Light-Responsiveness for Effective Degradation of Ibuprofen in Water

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KEYWORDS: g-C_3N_4; $NiCo_2O_4$; photocatalyst, PMS activation; Ibuprofen.

Herein, a 0D/3D $NiCo_2O_4$@g-C_3N_4 Z-scheme photocatalyst was successfully synthesized to degrade ibuprofen (IBP) in the photocatalytic system with the presence of peroxymonosulfate (PMS) under visible light. The 5% NiCo@CN exhibited the highest performance in IBP degradation among all catalysts and 96% IBP was degraded after 60 min. Experiments on IBP degradation also evaluated the impact of various conditions (PMS concentration, pH value, catalyst dosage, IBP concentration, and temperature). Scavenging tests and EPR analyses confirmed that the main reactive species for IBP degradation were h^+, $^1O_2$, and $SO_4^{\bullet -}$. The photocatalytic degradation of IBP resulted in a byproduct that was more benign than the parent compound. Experiments on cyclic degradation and analyses of fresh and used photocatalysts corroborated the remarkable stability of NiCo@CN. This study established a new framework for developing an effective photo-activator of PMS for cleaning up polluted environments.

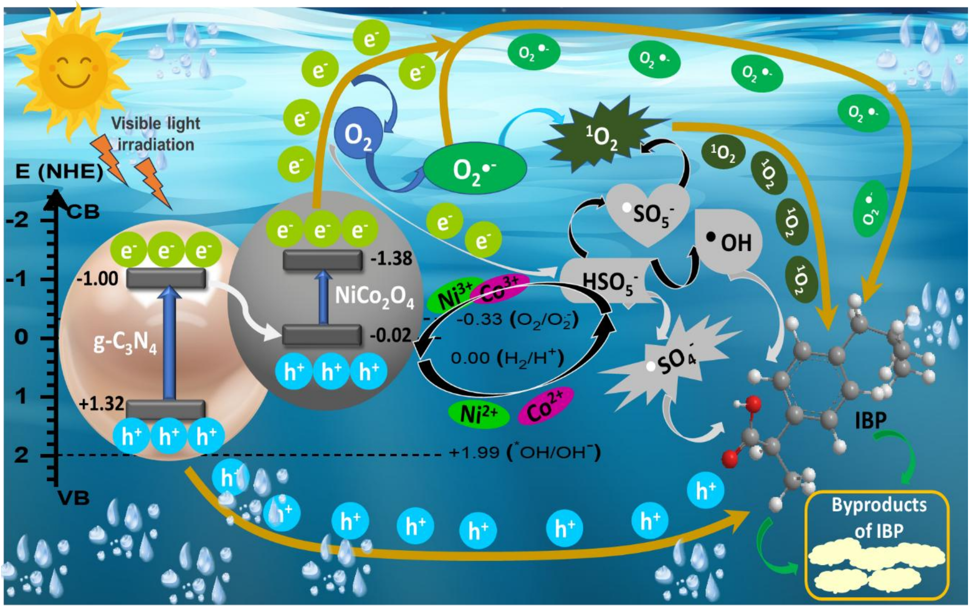

Figure 1. Illustraion of the photocatalytic activity of 0D/3D $NiCo_2O_4$@g-C_3N_4 Z-scheme photocatalyst.

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Acknowledgements: The author appreciates the kind financial assistance provided by the National Science and Technology Council (NSTC) Taiwan under grant number 111-2221-E-992-010.

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EEPM5-IL-027

INVITED SPEAKER 27

Photocatalytic Degradation of Green Bromocresol using TiO_2-Ag Coated Cork Ball: Structural and Morphological Analysis

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KEYWORDS: TiO_2-Ag; crystal structure; morphology; photodegradation; bromocresol green.

Photodegradation technology is an application that utilizes solar energy, which is inexhaustible, and does not require additional costs to obtain. Research on photodegradation technology indicates that contaminated water can be purified and produced into clean water. Titanium dioxide (TiO_2) is a semiconductor material that can be used as an application technology for photodegradation of organic pollutants. TiO_2 also has excellent photocatalytic activity, high stability, and non-toxicity. Silver (Ag) metal is used for doping, which acts as an excellent oxygen reduction cocatalyst. TiO_2 synthesis involves the sol-gel method with diethanolamine (DEA) as a solution stabilizer, and the cork ball substrate facilitates photodegradation technology, which can be applied using a dip coating fabrication method. This study aims to ascertain the crystal structure, morphology, and photodegradation applications of TiO_2-Ag variations in layer mass. The XRD results indicated an amorphous peak shape, attributed to the uneven surface of the foam ball and its small diameter. The SEM analysis revealed a diameter distribution from 140 nm to 260 nm. The photodegradation percentage of the bromocresol green (BCG) solution exhibited a direct correlation between the number of TiO2 layers and the degradation percentage. Cork balls coated with Ag paste demonstrated a higher degradation percentage than those without Ag paste. The highest degradation percentage was observed in the 4-layer TiO_2-Ag sample, reaching 69.36%, while the lowest was recorded in the 1-layer TiO_2-Ag sample, at 45.97%. This demonstrates that the TiO_2 layer is responsible for the observed increase in the value of the measured absorption. Specifically, it can be concluded that an increase in the thickness of the layer or the quantity of TiO_2 results in an increase in the absorption value. Consequently, the greater the number of layers, the higher the degradation percentage.

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Acknowledgements: The researcher expresses gratitude to the individuals who contributed to the completion of the article, particularly given its association with a research grant funded by Universitas Negeri Malang through the PNBP Grant number 19.5.955/UN32.20.1/LT/2022 for the NM Group.

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EEPM5-IL-028

INVITED SPEAKER 28

Development of Highly Efficient Ferrite-based Nanomaterials Photocatalytic Degradation of Pharmaceutical Pollutants

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KEYWORDS: Photocatalysis; $CuFe_2O_4$; Nanocomposites; Pharmaceutical contaminants; Water treatment.

The increasing presence of pharmaceutical pollutants in aquatic environments has promoted the development of advanced photocatalytic nanomaterials for efficient wastewater treatment. This study addresses the rational design and development of $CuFe_2O_4$-based nanomaterials as heterogeneous photocatalysts for the removal of recalcitrant pharmaceuticals. A series of heterogeneous $CuFe_2O_4$-based photocatalysts were synthesized, including bio-synthesized $CuFe_2O_4$, binary $CuFe_2O_4$/g-C_3N_4 nanocomposites, and ternary $CuFe_2O_4$/g-C_3N_4/MXene nanocomposites. The structural, morphological, optical, and surface properties of these nanomaterials were systematically characterized to gain insights into their physicochemical properties. The heterogeneous $CuFe_2O_4$-based photocatalysts were developed to exhibit improved photocatalytic activity and stability in photocatalysis and photo-Fenton processes, representing promising solutions for sustainable wastewater treatment.

The first part investigates the eco-friendly synthesis of $CuFe_2O_4$ nanoparticles (*bio*-$CuFe_2O_4$) using bio-reducers from plant wastes, including date pulp, date seeds, lemon peels, and pollen grains, via a sol-gel auto-combustion method. The synthesized $CuFe_2O_4$ catalysts were assessed in the photocatalytic degradation of ciprofloxacin in a peroxymonosulfate-assisted photo-Fenton system under UV-Vis irradiation. Among the different *bio*-$CuFe_2O_4$ catalysts, the date pulp-derived catalyst (*bio*-$CuFe_2O_4$/DP) exhibited the highest photocatalytic activity, achieving 97% ciprofloxacin degradation and 69.1% TOC removal. Additionally, the bio-CuFe2O4/DP catalyst demonstrated high stability and recyclability across multiple reaction cycles.

The second part focuses on the preparation of binary $CuFe_2O_4$/g-C_3N_4 nanocomposites for the photocatalytic degradation of nizatidine in a peroxydisulfate-assisted photo-Fenton system under visible LED irradiation. A novel flash heat treatment method was employed for the first time to synthesize 2D g-C_3N_4 with improved structural and optical properties. Binary nanocomposites were developed by using an ultrasound-assisted approach. The formation of an S-scheme heterojunction between the $CuFe_2O_4$ nanoparticles and the flash-heat-treated g-C_3N_4 structure significantly improved the charge carrier separation, leading to the complete removal of nizatidine within 43 min under LED light. Additionally, the binary $CuFe_2O_4$/g-C_3N_4 catalyst demonstrated excellent reusability, maintaining its high photocatalytic efficiency with minimal performance drop over several reaction cycles.

The third part presents a novel ternary $CuFe_2O_4$/g-C_3N_4/MXene nanocomposite for visible light photocatalysis, which achieved 96% degradation of ranitidine, with a reaction rate eight times higher than that of the binary $CuFe_2O_4$/g-C_3N_4. The incorporation of MXene significantly improved the photocatalytic efficiency by facilitating charge transfer through an S-scheme heterojunction, thereby suppressing electron-hole recombination and promoting the generation of ROS. Moreover, the

$CuFe_2O_4$/g-C_3N_4/MXene nanocomposite exhibited excellent reusability and high stability, and mechanistic studies confirmed the dominant role of hydroxyl and superoxide radicals in pollutant degradation.

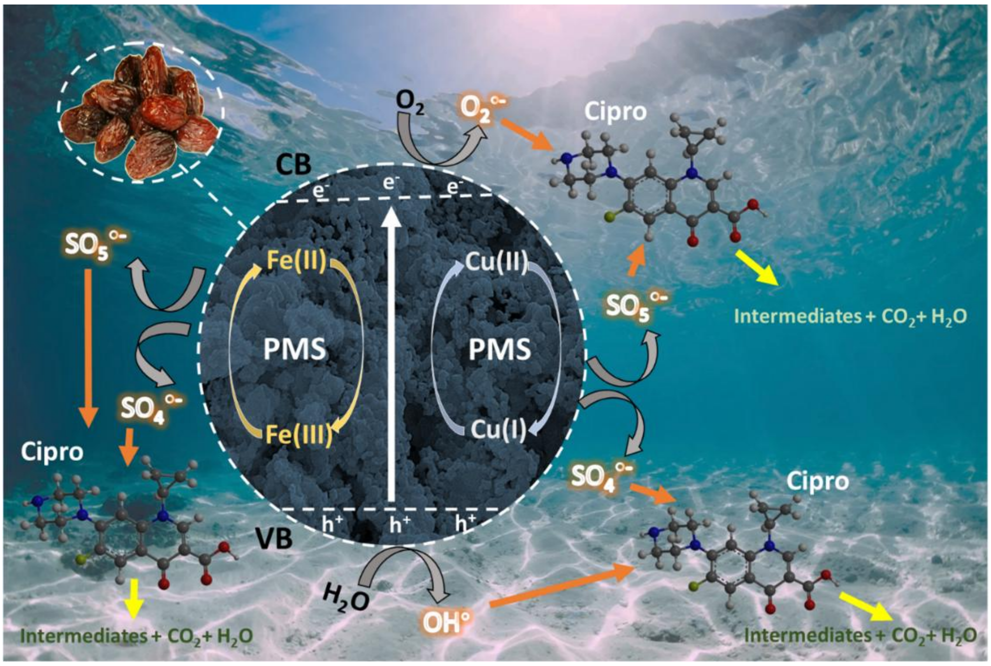

Figure 1. Schematic illustration of the working principle of developed photocatalyst.

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Acknowledgements: The authors thank Khalifa University of Science and Technology for the financial support through grant CIRA-2020-085.

Dr. **Mohammad Abu Haija** completed his Ph.D. in Chemistry in 2006 at the Technical University of Berlin in cooperation with the Fritz-Haber Institute of the Max Planck Society, Germany. Then, he worked as a postdoctoral fellow at Argonne National Laboratory, USA. Following that role, he worked in the Department of Chemistry at King Khalid University, Saudi Arabia. In 2012, Dr. Abu Haija joined The Petroleum Institute in the United Arab Emirates, which was later merged into Khalifa University. Dr. Abu Haija has received several Research Awards and served as the main advisor to 6 PhD students and 15 MSc students. His research group focuses on the design and synthesis of functional nanomaterials and their applications in catalysis, energy, and water treatment.

EEPM5-IL-029

INVITED SPEAKER 29

Facet Engineering of $SrTiO_3$ for Efficient Photocatalytic Reduction of Nitroaromatics

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KEYWORDS: Strontium Titanate; Euhedral Crystals; Nitroaromatics; Photocatalytic Organic Transformation

Photocatalysts such as TiO_2 are widely used in surface cleaning, disinfection, and environmental remediation applications. However, with relatively minor adjustments, such as the use of appropriate solvents, these materials can also facilitate selective organic transformations, including the photocatalytic reduction of nitroaromatic compounds [1]. This approach offers significant advantages in selectivity, particularly in the presence of other functional groups sensitive to reduction, as is often the case in pharmaceutical synthesis. For photocatalysis to become a viable alternative to conventional methods, it is essential to develop materials with sufficiently high quantum efficiencies. In this regard, strontium titanate ($SrTiO_3$) emerges as a promising candidate. Compared to TiO_2, $SrTiO_3$ is a milder oxidising agent and has been reported to achieve near-unity quantum efficiencies in photocatalytic water splitting [2].

Improving quantum efficiency can be achieved in various ways; however, most strategies ultimately focus on enhancing the separation of photogenerated charge carriers – electrons and holes. One promising approach involves crystal facet engineering, which facilitates anisotropic charge transfer by creating spatially separated sites for oxidation and reduction. We have demonstrated that this approach can effectively enhance the photocatalytic activity of anatase-TiO_2 [3].

In this work, we report the synthesis of well-faceted crystals of strontium titanate [4]. The high uniformity of the obtained samples allowed us to investigate how the presence of energetically distinct crystal facets influences charge separation. Our study reveals facet-dependent charge separation within the $SrTiO_3$ crystals, leading to the accumulation of electrons on the {001} facets, identified as the reduction sites, and holes on the {110} facets, serving as oxidation sites. Building on this understanding, we further demonstrated that photocatalytic activity can be enhanced by decorating the crystals with metal nanoparticles. We examined the effect of metal type on activity and the role of selective deposition on specific crystal facets. We will present how tuning the crystal facets and controlling the spatial distribution of metal nanoparticles can significantly enhance the photocatalytic efficiency of $SrTiO_3$.

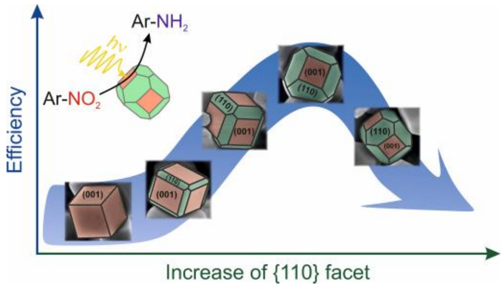

Figure 1. Effect of tailored $SrTiO_3$ crystal on the efficiency of photocatalytic reduction of nitroaromatics.

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Acknowledgements: The authors acknowledge the support of the National Science Centre within the OPUS23 project (2022/45/B/ST5/04087).

Marcin Kobielusz earned his bachelor's degree in chemistry from Jagiellonian University in Kraków, where he also completed his master’s thesis in 2012. That same year, he began doctoral studies under Prof. Wojciech Macyk. Between 2012 and 2015, Marcin worked as a contractor on the FNP TEAM project. In 2013 and 2014, he gained international experience through internships at the University of Bari, Italy. He defended his doctoral dissertation with distinction in 2016 and then served as an assistant at Jagiellonian University (2016–2018). In 2019, he was a visiting researcher at Western Sydney University. He was a postdoc in the TEAM project. He is currently an assistant professor at Jagiellonian University.

EEPM5-IL-030

INVITED SPEAKER 30

Oxygen-Doped g-C_3N_4 Integrated with In_2S_3 Quantum Dots: A Tailored n–n Heterojunction Photocatalyst for Visible-Light-Driven Antibiotic Degradation

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KEYWORDS: Photocatalysis; Advanced Functional Materials; Environmental remediation; Advanced Oxidation Process; Materials Synthesis

Antibiotic residues entering water systems threaten ecosystems and human health primarily because these compounds resist breakdown, can concentrate in living tissues, and fuel the global spread of resistance genes. Metronidazole (MDZ), an antiprotozoal of the nitroimidazole class, exemplifies the issue, commonly traced in effluent and receiving waters in concentrations that resist typical treatment. Owing to its complex and prolonged environmental toxicity, strategies that sustainably and efficiently remove MDZ residues are urgently needed. Photocatalytic advanced oxidation processes (AOPs) operating under sunlight can, in principle, break down MDZ by harnessing ambient irradiation to drive oxidative fragmentation. A recent advance in this field, persulfate (PS)-based photocatalytic oxidation, elevates the oxidizing potency of AOPs. When included in reactions, the PS under sunlight and laboratory-visible light becomes a surrogate electron acceptor that generates abundant reactive sulfate radicals, achieving advanced and sustained photocatalytic degradation of MDZ.

This work demonstrates the design and synthesis of In_2S_3 quantum dots (QDs) anchored on oxygen-doped g-C_3N_4 via an ultrasonication process to form In_2S_3/O@g-C_3N_4 heterojunction photocatalyst [1]. The complete characterization analysis of the material inferred the successful dispersion of In_2S_3 QDs (average size ~ 6.62 nm) onto the O@g-C_3N_4 matrix and confirmed the interfacial contact needed for heterojunction formation. A series of control experiments at optimal conditions of the activated PS system with 0.24 g/L of catalyst dosage, 15 mg/L of MDZ under 25 minutes of visible light irradiation was carried out to analyze the synergistic effect of each component. The pristine g-C_3N_4 showed 21.4% efficiency, while oxygen doping enhanced the performance to 46.4% and In_2S_3 exhibited an effective 34.9% for the removal of MDZ. However, In_2S_3/O@g-C_3N_4 photocatalyst exhibited 98.2% degradation efficiency due to the formation of n-n heterojunction, leading to enhanced charge transfer and reduced charge recombination. In addition, the S-scheme charge transfer pathway, where the equilibrium of Fermi levels between In_2S_3 and O@g-C_3N_4 develops an internal electric field that helps efficient charge separation while preserving strong redox potentials at the interface. Reactions using hydroxyl and superoxide quenchers confirmed that reactive oxygen species (ROS) play primary roles, while LC-MS profiling revealed key transformation intermediates and essential degradation pathways that guide the complex MDZ molecule to simple end-products. Notably, the same photocatalyst achieved rapid, consistent oxidation of a wide range of emerging pollutants, extending its relevance to contaminants beyond conventional pharmaceuticals. Parallel reductions in chemical oxygen demand (COD) and total organic carbon (TOC) reinforced the

conclusion that oxidation progresses to complete mineralization. Furthermore, its high reusability up to seven cycles, maintaining around 75% efficiency, confirmed the structural stability and durability. In summary, the near-complete photodegradation of MDZ by n-n heterojunction-based $In_2S_3/O@g\text{-}C_3N_4$ photocatalyst was attributed to the structural synergy, effective PS-activation, and improved charge-carrier dynamics (**Figure 1**). Besides, the S-scheme charge transfer mechanism paved the way for removing a broad range of toxic pollutants.

The future work will focus on integrating kinetic modelling studies into photocatalytic systems to gain predictive control, minimize energy and reagent input, optimize reaction (operational) conditions, and gain deeper insights into reaction mechanisms [2, 3]. Hence, this modelling will act as a guide to scale up the photocatalytic system for industrial-scale water treatment applications, leading to a highly efficient AOP for emerging contaminant removal.

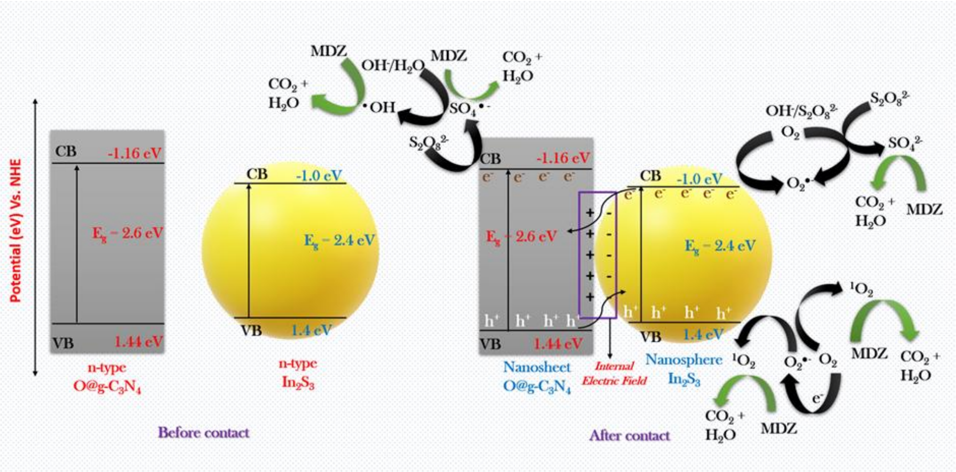

Figure 1. Charge transfer dynamics of the fabricated $In_2S_3/O@g\text{-}C_3N_4$ heterojunction photocatalyst.

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Acknowledgements: This work is supported by the MoE, India, funding program of the National Institute of Technology Silchar, India, and by the Research and Development Program of Ghent University Global Campus (GUGC), South Korea.

Dr. **Soumya Ranjan Mishra** is a postdoctoral researcher at the Center of Green Chemistry and Biotechnology, Ghent University Global Campus, South Korea, mentored by Prof. Dr. ir. Philippe M. Heyndericks. Specializing in material synthesis for environmental remediation, he has published impactful research in prestigious journals and is distinguished among the top 2% of scientists by Elsevier and Stanford University. He completed his Ph.D. at the National Institute of Technology Silchar, receiving the gold medal for best doctoral thesis in 2024. His current work advances innovative remediation technologies and strengthens the scientific community through global collaborations.

EEPM5-IL-031

INVITED SPEAKER 31

CuS and Ag Integrated Sb_2O_3 Nanosheets: Formation, Charge Transfer Enhancement and Investigation for Photocatalytic Decontamination of Organic Pollutants

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KEYWORDS: Photocatalyst; Ag@ Sb_2O_3/CuS; Rhodamine B; Ciprofloxacin; Recombination.

Ag@Sb_2O_3/CuS heterojunctions were created with varied amount of CuS on Sb_2O_3 nanosheets (2, 3 & 4 wt%) and Ag on optimized Sb_2O_3/CuS (2, 3, & 4 wt%) via hydrothermal method and deposition method respectively (Fig. 1) [1, 2]. Photocatalysts were analyzed for their optical properties, morphological characteristics, crystalline structures, dynamics of charge recombination, chemical compositions and surface charge [3 – 6]. Photocatalytic performance of constructed materials was examined on Rhodamine B (RhB) dye and ciprofloxacin (CP) antibiotic in illumination of visible light. Ag(3wt%)@Sb_2O_3/CuS(3wt%) exhibited highest photocatalytic decontamination efficiency i.e., 86.39% in 180 min for CP and 90.16% in 140 min for RhB at highest rate constant (k) of 0.0095 min^{-1} for CP and 0.0102 min^{-1} for RhB. This is owing to the formation of heterojunction in Sb_2O_3/CuS which facilitate effective separation of charges and increase light harvesting, thus boost efficiency [7 – 9]. Furthermore, subsequent deposition of Ag on Sb_2O_3/CuS boosts photocatalytic performance to a higher extent owing to localized surface plasmon resonance (LSPR) [10]. $^{\bullet}OH$ and $^{\bullet}O^{2-}$ were recognized as active species in both the removal of CP and RhB. Also, Ag (3 wt%) @ Sb_2O_3/CuS (3 wt%) photocatalyst displayed outstanding stability after five runs, in which efficacy dropped by 4.4% for RhB and 5.3% for CP only. Electrochemical analysis [11] as executed by EIS and Cyclic Voltammetry which supported lower charge resistance after the construction of nanocomposite.

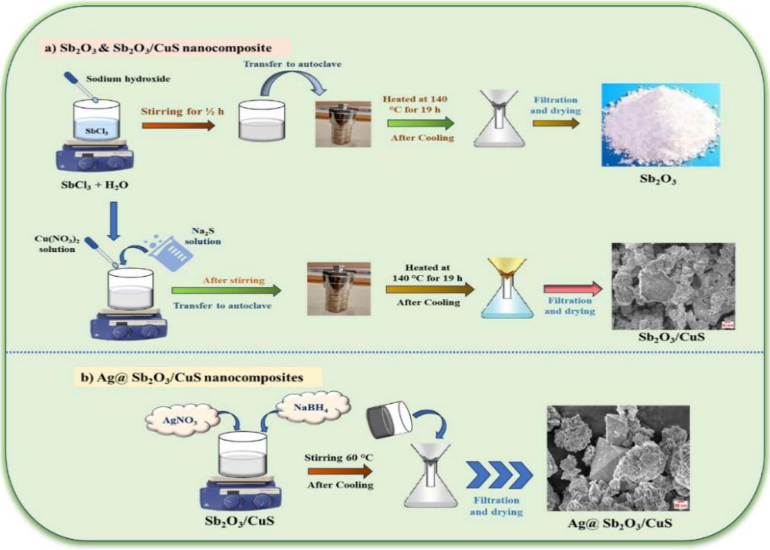

Fig.1. Schematic diagram of fabrication method of (a) Sb_2O_3 & Sb_2O_3/CuS nanocomposite and (b) Ag@Sb_2O_3/CuS nanocomposite.

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Acknowledgements: Shruti Jain thanks CSIR-New Delhi, India for Senior Research Fellowship. Naveen Kumar thanks M. D. University Rohtak for the Post Seed Grant (2022-2025) and the characterization facilities by the ACIL, M. D. University Rohtak

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EEPM5-IL-032

INVITED SPEAKER 32

Optimizing Plasma-assisted Reactive Thermal Evaporation Growth of In_2O_3 and Its Nanostructured Composites for Enhancing Hydrogen Production via Water Splitting

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KEYWORDS: Indium oxide; Tungsten oxide & nitride; Nanocomposite; Nanowires; Reactive plasma-assisted; Water-splitting

Recently, visible light-driven semiconducting photocatalysts for hydrogen production have attracted considerable attention from both the scientific community and industry. Among them, indium oxide (In_2O_3) is a promising semiconductor; however, its relatively wide bandgap of approximately 3.75 eV falls within the ultraviolet region, which limits its photocatalytic efficiency under visible light. Consequently, extensive research efforts have focused on modifying In_2O_3 to narrow its bandgap and enhance its activity in the visible spectrum. In this study, plasma-assisted reactive thermal evaporation (PARTE) was employed to synthesize In_2O_3 and its nanostructured composites. Process optimization was carried out to improve their hydrogen generation performance. A range of morphologies and composite structures were fabricated, including intrinsic In_2O_3, In_2O_3/WO_3, W_2N/In_2O_3, as well as nanorods, nanowires, and faceted nanostructures. The incorporation of WO_3 and W_2N into the In_2O_3 matrix significantly reduced the optical bandgap, shifting it into the visible light region (2.71–1.69 eV, corresponding to 460–700 nm). Among these, the W_2N/In_2O_3 nanostructures and nanowires exhibited substantially enhanced visible-light photocurrent densities of 1.84 mA/cm² and 3.80 mA/cm² at 1 V vs. Ag/AgCl, with corresponding bandgaps of 2.58 eV and 2.4 eV, respectively. Notably, heavy nitrogen doping (~55 at%) into the In_2O_3 crystal lattice further reduced the optical bandgap to 2.53 eV, resulting in a significant increase in photocurrent density to 7.91 mA/cm² at 1 V vs. Ag/AgCl. These findings suggest that forming nanocomposites or employing high levels of nitrogen doping effectively improves visible light absorption, enhances charge separation, and aligns the band structure more favourably with the redox potentials of the Normal Hydrogen Electrode (NHE), thereby boosting overall photocatalytic performance.

Prof. **Boon Tong Goh** is a professor in the Department of Physics, Universiti Malaya, and currently serves as Deputy Dean at the Institute for Advanced Studies and Deputy Head of the Low Dimensional Materials Research Center. His research focuses on nanomaterials, including 1D and 2D structures, metallic nanoparticles, and nanostructured thin films. He has received numerous prestigious awards, such as the Newton Advanced Fellowship and TRSM Award. Dr. Goh holds various academic roles globally, including adjunct and visiting professorships, editorial positions, and PhD examiner appointments. He has published nearly 250 peer-reviewed papers with 3,660 citations (h-index = 31) and is recognized internationally for his contributions to nanomaterials research.

EEPM5-IL-033

INVITED SPEAKER 33

Bridging Material Modifications with Kinetic Modelling for Optimal Performance in Advanced Photocatalysis

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KEYWORDS: Photocatalysis; Material synthesis; Kinetic modeling; DFT analysis, Oxygen vacancies

This presentation demonstrates how material modifications, together with kinetic modeling, enhance photocatalytic performance and clarify reaction mechanisms for process scale-up. The optimization of photocatalytic processes requires a dual understanding of material design and reaction dynamics. Fabricating bandgap-engineered photocatalysts is a novel strategy to overcome the challenges posed by conventional semiconductor materials for photocatalytic processes triggered by solar energy [1]. The impact of oxygen-vacancy-rich semiconductor nanostructures on the performance of the photocatalyst and its mechanistic aspect is analyzed in this presentation. The presence of oxygen vacancies within the lattice not only decreased the photogenerated charge carrier traps, thus improving the carrier lifetime, but also improved the electronic band structure owing to the enhanced light absorption in the bandgap [2]. Also, these defect levels increased the adsorption energy for surface reactions and thus increased the efficiency of surface redox reactions for producing reactive oxygen species. The resulting oxygen-vacancy-rich photocatalyst performed significantly better than its pristine counterpart by combining defect-mediated electronic tuning with optimized synthesis conditions [3]. This suggests that oxygen vacancy engineering is a flexible approach for next-generation photocatalytic materials.

While photocatalysis is widely recognized as a promising green technology for water and wastewater treatment, its practical implementation is often hindered by the complexity of underlying reaction pathways. The overall degradation rate results from multiple concurrent phenomena, including adsorption of contaminants on the catalyst surface, photogeneration of electron–hole pairs, radical-mediated reactions in the liquid phase, and recombination losses. Traditional kinetic approaches, such as pseudo-first-order models, can capture apparent degradation trends but fail to resolve the contributions of these individual processes. Developing comprehensive kinetic models is therefore crucial not only for interpreting laboratory-scale experiments but also for enabling predictive simulations and guiding scale-up to pilot and industrial systems [4].

In order to obtain deeper insights into the photocatalytic degradation mechanism, we developed a kinetic model that incorporates both reversible adsorption and photocatalytic degradation, while distinguishing between two concurrent pathways: (i) surface-mediated degradation initiated by electron–hole pairs and (ii) solution-phase degradation driven by hydroxyl radicals. Importantly, as illustrated in Figure 1, the model integrated the dissociation equilibria of contaminants as a function of pH, which determined both adsorption affinity and reactivity. Under acidic conditions, protonated molecules showed higher surface adsorption, and degradation occurred primarily via electron–hole interactions at the catalyst interface. At higher pH, however, the deprotonated species exhibited lower adsorption affinity, but degradation accelerated due to the increased formation of hydroxyl radicals, which attack pollutants in the solution phase [5]. These findings were further supported by DFT analysis and electrostatic potential (ESP) maps (Figure 1c and 1d), which elucidated the tendency for higher degradation rates of cationic dyes under basic conditions and anionic dyes under acidic conditions. Additionally, the model was adapted in another investigation to analyze the simultaneous degradation of a dye mixture consisting of methylene blue and methyl orange, while also considering the sensitization effect of methylene blue on the ZnO catalyst. Through this approach, the model enabled us to quantify the relative contributions of charge carriers generated directly by the catalyst compared to those produced via the dye-sensitization pathway [6].

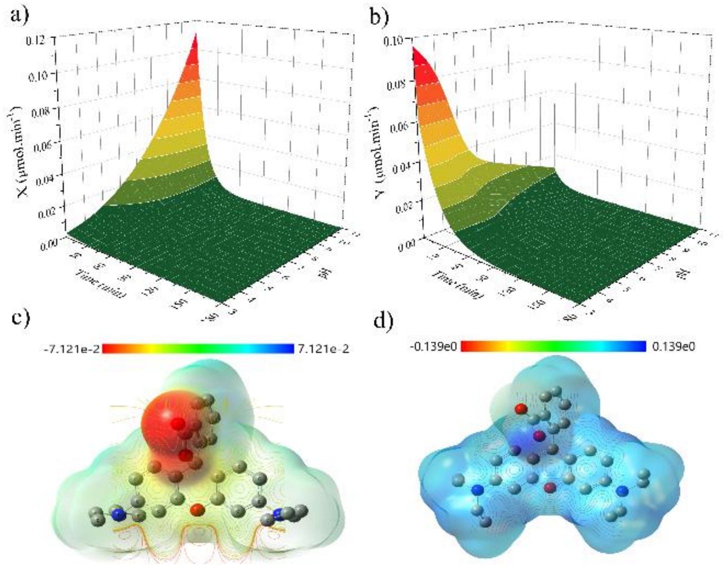

Figure 1. Simulations of a) photocatalytic degradation of rhodamine B (RhB) in the solution, b) photocatalytic degradation of RhB on the catalyst surface, c) ESP of neutral RhB, and d) ESP of protonated RhB.

Specifically, application of the kinetic model revealed that introducing oxygen vacancies into ZnO increased the adsorption equilibrium coefficient of thiabendazole from 1.49 10^4 L/mol in the pristine catalyst to 2.39 10^4 L/mol in the reduced catalyst, and the degradation rate coefficients in both the solution phase and on the catalyst surface respectively increased by ~34% and ~104%, following the introduction of oxygen vacancies.

In conclusion, the complementary combination of material modification (and its understanding from characterization) and kinetic modeling (in its fundamental nature in terms of elementary steps) is necessary in advancing photocatalytic water treatment. While material design enhance photocatalytic activity by narrowing the bandgap and stabilizing charge carriers, it is the comprehensive kinetic modeling framework that provides a mechanistic understanding of how these defects, together with environmental factors such as pH, govern photocatalytic performance. By capturing reversible adsorption, contaminant dissociation, and simultaneous surface- and solution-phase reactions, the model not only describes laboratory behavior with high accuracy but also offers a predictive tool for reactor simulations and process scale-up. The dual approach – catalyst engineering combined with mechanistic modeling (including DFT) – forms the indispensable foundation for designing efficient and scalable photocatalytic systems for real-world water treatment applications.

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Prof. **Philippe M. Heynderickx** earned his Civil Chemical Engineer degree in 2004 and his PhD in Chemical Technology in 2009, focusing on heterogeneous catalysis (modelling via experimental data). Since 2015, he has been a professor at Ghent University Global Campus (South Korea), specializing in photocatalysis for pollution remediation, including indoor air cleaning and water purification. He works on catalyst synthesis, characterization and in-depth modelling of photocatalytic processes to improve environmental applications. He is also active in the field of hydrothermal carbonization for upgrading waste into hydrochar (adsorbent material) and activated carbon (adsorbent, catalyst carrier material…). He has authored over 100 publications with extensive international recognition. He received the Young Scientist Award at the 2008 ICC Seoul.

EEPM5-IL-034

INVITED SPEAKER 34

Impact of Surface Treatment on Charge Carrier Dynamics in Bi_4NbO_8Cl Photocatalysts Probed by Ultrafast Time-Resolved Absorption Spectroscopy

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KEYWORDS: Layered oxyhalide, Photocatalyst, Time-resolved absorption spectroscopy

Bi_4NbO_8Cl (BNOC) is a photocatalytic material belonging to the layered oxyhalide family that is capable of driving water splitting reaction under visible light illumination. By tuning its chemical composition or layered structure, the electronic properties of the material – such as its band structure and defect states – can be modified to better suit specific application. In the context of photocatalytic water splitting, such modifications often lead to an enhancement in photocatalytic activity. Owing to this versatility, BNOC continues to draw in considerable attention in the field of photocatalysis [1].

It is well established that many photocatalysts are incapable of driving the hydrogen (H_2) evolution reaction on their own, or in other cases, can do so but with low efficiency. To overcome this limitation, deposition of co-catalyst has proven to be an effective strategy to spur or enhance H_2 evolution. Among them, Platinum (Pt) is widely known for its notorious efficiency as a H_2 evolution co-catalyst. Owing to its innately high work function, Pt readily functions as an electron sink and provides reaction sites for reduction reactions. However, charge transfer to Pt is not limited to electrons. In certain cases, holes have also been reported to migrate toward Pt [2]. This can lead to the undesirable phenomenon of Pt particles becoming recombination centers which diminishes photocatalytic performance. Hence, suppressing holes transfer to Pt is a critical consideration in the design of photocatalytic systems.

Recently, Ogawa et. al. discovered that implementation of surface treatment on BNOC drastically enhances its H_2 evolution activity in the presence of Pt. Nevertheless, how such treatment alters the dynamics of the photogenerated electrons and holes remains unclear. In this work, we delved into this aspect by conducting time-resolved absorption spectroscopy (TAS) spanning both femto- and microsecond timescales. The decay kinetics of photoexcited electrons and holes in untreated and surface-treated BNOC, with and without Pt deposition, were analyzed. It was found that surface treatment not only prolonged the lifetime of photogenerated charge carrier, it also enhanced the rate of electrons transfer to Pt. Holes transfer to Pt was also observed, however the rate was revealed to be notably lower than electrons transfer, and was also unaffected by surface treatment. We believe these effects collectively contributed to the improved photoactivity, and the details of the charge carrier dynamics observed through TAS will be discussed.

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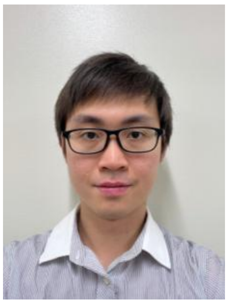

Dr. **Yi-Hao Chew** is a specially-appointed assistant professor at Okayama University, Japan, specializing in ultrafast time-resolved spectroscopy of photocatalytic materials. Building on four years of experience in engineering photocatalysts for enhancement of activity in water splitting reaction, his current research investigates the fundamental charge carrier dynamics that govern the photocatalytic performance. By integrating the knowledge from empirical materials development with advanced spectroscopic techniques, his work aims to deliver mechanistic insights that inform the rational design and optimization of next-generation photocatalytic materials. Chew holds a PhD from Monash University Malaysia and has published a series of works spanning materials synthesis to fundamental mechanistic studies.

EEPM5-IL-035

INVITED SPEAKER 35

Integrating Kinetic Modelling and DFT Analysis to Elucidate Phenol Degradation over TiO_2 Photocatalysts

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KEYWORDS: Photocatalysis; Phenol degradation; Beer–Lambert law; Kinetic modelling; DFT analysis

Photocatalytic degradation has emerged as one of the most promising strategies for the removal of persistent organic pollutants from water, yet the fundamental aspects controlling its efficiency remain underexplored [1]. In particular, the interplay between the light absorption of target compounds and the fate of aromatic intermediates has received limited attention, despite their crucial role in determining degradation kinetics and mechanisms. In this study, we investigate the photocatalytic degradation of phenol as a model contaminant over two benchmark TiO_2 photocatalysts (P25 and UV100) under both UVA and UVC irradiation. By carefully monitoring phenol conversion and the evolution of key aromatic intermediates including catechol, hydroquinone, and trihydroxybenzene, we provide a detailed picture of the degradation pathway and the conditions that favor the accumulation or further transformation of intermediates [2]. Figure 1 indicates the phenol degradation pathway and the corresponding kinetic parameters for each step.

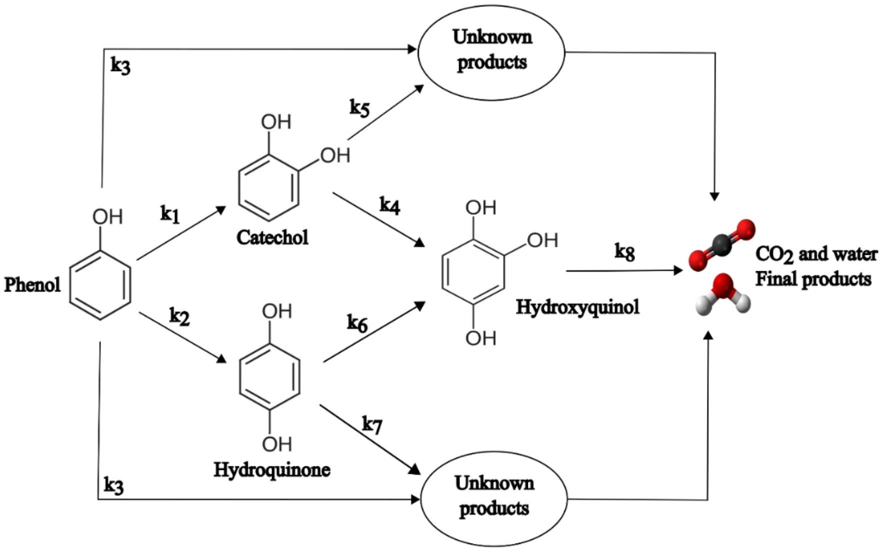

Figure 1. Degradation pathway of phenol and its corresponding rate coefficients.

To quantitatively interpret the experimental results, we developed a kinetic model that incorporates both light absorption processes by the contaminants and intrinsic photocatalytic reaction steps [3]. The Beer–Lambert law was explicitly applied to account for light attenuation by phenol and its aromatic intermediates, a factor often neglected in conventional photocatalytic kinetic models. This framework enabled accurate prediction of pollutant degradation and intermediate formation across a wide range of initial phenol concentrations. The results reveal that the light absorption properties of phenol itself strongly influence the apparent degradation kinetics, particularly at high pollutant concentrations, where the competition between photon absorption by the substrate and the catalyst becomes decisive.

Complementary Density Functional Theory (DFT) calculations were employed to probe the hydroxylation pathways of phenol and to assess the relative reactivity of its intermediates. Mulliken atomic charge analysis was used to identify the most electron-rich carbon sites in phenol, thereby explaining why hydroxylation preferentially occurs at specific positions to yield catechol and hydroquinone as the dominant primary intermediates. These theoretical insights confirmed the experimental observation of their preferential formation, owing to favorable electronic structures and strong interactions with hydroxyl radicals. The analysis further rationalized the delayed formation of trihydroxybenzene, which arises as a secondary product once the primary intermediates are depleted. Overall, the results establish a clear link between molecular electronic properties, hydroxylation site selectivity, and observed degradation kinetics [4].

In conclusion, this combined experimental–theoretical approach provides a comprehensive framework for understanding photocatalytic degradation pathways and the factors that control them [5]. By highlighting the significance of pollutant light absorption in shaping both efficiency and mechanism, this work advances the design of predictive kinetic models and demonstrates their value in bridging laboratory-scale studies with practical water treatment applications. The insights gained are expected to guide the development of more efficient photocatalytic systems and contribute to their translation into large-scale processes for environmental remediation.

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Acknowledgements: The authors acknowledge the Research and Development Program of Ghent University Global Campus (GUGC), South Korea.

Dr. **Alireza Ranjbari** received his PhD from Ghent University in 2024. He is currently a postdoctoral researcher and teaching assistant at the Center for Green Chemistry and Environmental Biotechnology, Ghent University Global Campus, South Korea. His research focuses on photocatalysis for the removal of contaminants from water and air. He also works on photocatalytic hydrogen production, CO_2 reduction, and the application of machine learning to interpret and optimize experimental photocatalysis results. He specializes in comprehensive kinetic modeling and simulation of photocatalytic degradation processes, aiming to bridge experimental studies with theoretical insights to advance sustainable environmental and energy technologies.

EEPM5-CT-001

CONTRIBUTING TALK 1

Atomic-Level Interface Design Enabling Ultrafast Charge Separation and Transfer for Photocatalytic H_2 Evolution

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KEYWORDS: Superlattice interface; S-scheme heterojunction; $Mn_{0.5}Cd_{0.5}S$; Photocatalytic H_2 evolution; Ultrafast charge separation

The rapid recombination of photoinduced charge carriers in semiconductors fundamentally limits their application in photocatalysis. Herein, we report that a superlattice interface and S-scheme heterojunction based on $Mn_{0.5}Cd_{0.5}S$ nanorods can significantly promote ultrafast charge separation and transfer. Specifically, the axially distributed zinc blende/wurtzite superlattice interfaces in $Mn_{0.5}Cd_{0.5}S$ nanorods can redistribute photoinduced charge carriers more effectively when boosted by homogeneous internal electric fields and promotes bulk separation. Accordingly, S-scheme heterojunctions between the $Mn_{0.5}Cd_{0.5}S$ nanorods and $MnWO_4$ nanoparticles can further accelerate the surface separation of charge carriers via a heterogeneous internal electric field. Subsequent capture of the photoelectrons by adsorbed H_2O is as fast as several picoseconds which results in a photocatalytic H_2 evolution rate of 54.4 $mmol \cdot g^{-1} \cdot h^{-1}$ without any cocatalyst under simulated solar irradiation. The yields are increased by a factor of ~5 times relative to control samples and an apparent quantum efficiency of 63.1% at 420 nm is measured. This work provides a protocol for designing synergistic interface structure for efficient photocatalysis.

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Sijie Wan is currently pursuing his Ph.D. under the supervision of Researcher Shaowen Cao at Wuhan University of Technology. His primary research focuses on the design and synthesis of atomic-level photocatalytic structures, as well as first-principles theoretical calculations. The photocatalytic materials he designs and synthesizes are mainly applied in fields such as photocatalytic water splitting for hydrogen production, CO_2 photoreduction, and multifunctional artificial photosynthesis. Additionally, he conducts in-depth investigations into the structure–activity relationships between atomic-level structures and their performance. He has published three papers as the first author or co-first author in journals including Nature Communications, Rare Metals, and Interdisciplinary Materials.

EEPM5-CT-002

CONTRIBUTING TALK 2

Pivotal Role of Light in Photothermocatalytic CO_2 Reduction by Methane on Supported Nanostructured Group VIII Metals

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KEYWORDS: Photothermocatalysis; CO_2 reduction; Hydrogen production

The escalating reliance of the modern industrialization process on fossil fuels has not only exacerbated the global energy scarcity, but also triggered environmental deterioration problems centered on excessive greenhouse gas emissions. Converting CO_2 into solar fuels via photocatalysis using solar energy offers a promising solution to these challenges. Nevertheless, the photocatalytic CO_2 reduction is hindered by its low light-to-fuel efficiency (η) and fuel production rate (r_{fuel}). Therefore, developing a new strategy to substantially enhance η and r_{fuel} remains an urgent yet challenging task. Recently, we developed a photothermocatalytic approach for CO_2 reduction by methane (DRM) employing various catalysts composed of nanostructured group VIII metals supported on metal oxides, including Pd nanoparticles supported on Co and Al co-doped MgO (η = 25.3%, r_{H2} = 73.04 mmol min^{-1} g^{-1}), Ni nanoparticles supported on Ni and Y co-doped Al_2O_3 (η = 29.2%, r_{H2} = 76.79 mmol min^{-1} g^{-1}), Ni nanoparticles supported on Ni and Sr co-doped Al_2O_3 (η = 30.6%, r_{H2} = 114.2 mmol min^{-1} g^{-1}), as well as Pd nanoparticles, Ni nanoparticles and highly dispersed Ni supported on Al_2O_3 (η = 25.4%, r_{H2} = 82.87 mmol min^{-1} g^{-1}). Under focused UV-vis-IR and vis-IR illumination, the photothermocatalytic strategy demonstrates remarkably high r_{fuel} and η. The approach follows a light-driven thermocatalytic DRM mechanism. Interestingly, the focused light not only provides the necessary thermal energy, but also induces a photoactivation effect, markedly enhancing catalytic activity, which distinctly differs from photocatalysis on semiconductor photocatalysts. Through extensive experimental evidences, we put insight in the photoactivation for DRM on the nanostructured group VIII metal catalysts.

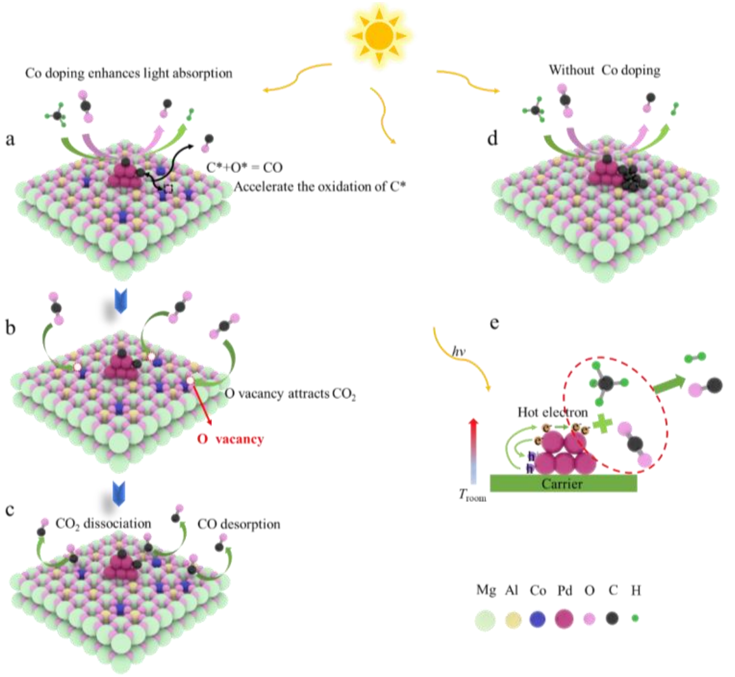

Figure 1. Schematic diagram of photothermocatalytic DRM over Pd nanoparticles supported on Co and Al co-doped MgO.

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Acknowledgements: The authors thank National Natural Science Foundation of China (21972109, 21673168) for awarding the grant.

Lei Ji is a Ph.D. candidate at Wuhan University of Technology. Her present interest involves photothermocatalytic CO_2 reduction.

EEPM5-CT-003

CONTRIBUTING TALK 3

Photocatalytic Upcycling of PET Plastic Waste Integrated with H_2 Generation Driven by Cadmium Indium Sulfide/Cobalt Oxide Catalysts

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KEYWORDS: plastic waste upcycling; photocatalysis; p-n heterojunctions; $Cd_2In_2S_5$ photocatalysts; hydrogen

Energy crisis remains a stern global issue to date, which is attributed to the rapid development of society and the increasing human population. In the quest for a sustainable future, artificial photosynthesis arises as one of the promising but arduous approaches to utilize sunlight as an energy source for clean energy production under benign conditions. Unlike the natural photosynthesis process, a variety of energy conversion reactions, such as H_2O splitting, CO_2 reduction, and N_2 fixation, that occur in artificial photosynthesis can be applied via a semiconductor with rising solar-to-chemical efficiency. Unlike the natural photosynthesis process, a variety of energy conversion reactions, such as H_2O splitting, CO_2 reduction, and N_2 fixation, that occur in artificial photosynthesis can be applied via a semiconductor with rising solar-to-chemical efficiency [1-4]. Particularly, the H_2O splitting is often restrained by the oxygen evolution reaction (OER) owing to the sluggish kinetics and high thermodynamic barriers. Thus, the introduction of sacrificial agents is a typical way of driving the oxidation half-reaction, yet it is not economically viable for larger-scale applications and does not fully utilize both half-reactions for concurrent redox processes. Different from using the sacrificial reagents, the oxidation of simple organic molecules that is more kinetically favorable can replace OER to consume photoinduced holes to improve the overall efficiency of the photocatalytic reaction [5, 6]. In this regard, the photocatalytic H_2 generation coupled with plastic transformation using semiconductors offers a novel approach to address energy challenges and contemporary environmental issues for achieving a more sustainable and eco-friendly future. In this work, an n-p heterojunction $Cd_2In_2S_5/Co_3O_4$ composite with a built-in electric field is engineered to convert an omnipresent plastic, namely polyethylene terephthalate (PET), into H_2 (63.10 $\mu mol\ h^{-1}$) and carboxylates (formic acid: 8.34 $\mu mol\ h^{-1}$; oxalic acid: 1.22 $\mu mol\ h^{-1}$; glycolic acid: 5.22 $\mu mol\ h^{-1}$) under visible light irradiation. The solar-to-hydrogen and apparent quantum efficiency in this sacrificial-substrate-free system achieve a value of 0.17% and 0.48% (420 nm), respectively. The excellent performance is primarily accredited to the expanded light absorption range, enhanced specific surface area, improved carrier separation efficiency, and boosted interfacial charge transport. Advanced characterization techniques, including KPFM and EPR, uncover the intricate charge transfer dynamics of PET photoreforming, where the photogenerated holes accumulated on Co_3O_4 initiate the plastic oxidation half-reaction. Finally, the photoreforming of real-world PET bottles demonstrates the broad universality of $Cd_2In_2S_5/Co_3O_4$ hybrids. This research presents a trailblazing standpoint for the design of p-n heterojunctions to bridge new exemplifications toward environmental sustainability.

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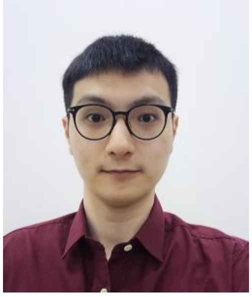
Ke Ming Lim received his Bachelor of Chemical Engineering with Honors from Xiamen University, Malaysia, in 2023. He is currently pursuing a Master's degree under the supervision of Prof. Dr. Wee-Jun Ong at Xiamen University Malaysia. His research topic of interest focuses on the design of nanostructured photocatalysts and the transformation of plastic waste into high-value products via artificial photosynthesis to realize the idea of "Waste-to-Wealth".



EEPM5-CT-004

CONTRIBUTING TALK 4

Key Role of Light in Light-Promoted Photothermocatalytic Cellulose Steam Reforming to Syngas on Ni/La^{3+}-doped CeO_2

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KEYWORDS: Photothermocatalysis; Cellulose steam reforming; Green syngas production

Against the backdrop of increasing global energy demand, the search for alternatives to fossil fuels has become an urgent need. Syngas (H_2 and CO) has attracted attention as a potential future energy carrier, which can be used not only as a direct fuel, but also converted into liquid fuels through processes such as Fischer-Tropsch synthesis. Photothermocatalytic cellulose steam reforming offers a sustainable pathway for syngas production from renewable biomass resources. However, a significant challenge in complex biomass reforming reactions is the formation of excess tar and severe char, which results in low syngas yields and compromises catalytic stability. Recently, we reported a light-driven photothermocatalytic approach for cellulose steam reforming using Ni nanoparticles supported on La^{3+}-doped CeO_2 catalysts, which highly enhanced H_2 and CO production rates and light-to-fuel efficiency while reducing byproducts (for details see Table 1). Characterization techniques reveal that a synergy between enhanced H_2O absorption capacity due to increased oxygen vacancies and intrinsic lattice oxygen activation is provided by La^{3+} doping, which is responsible for the extraordinary catalytic performance of Ni/Ce_3La_1. Significant photoactivation was found in accelerating the oxygen migration from both ceria lattice and H_2O adsorbed on oxygen vacancies, particularly promoting the conversion of H_2O with byproducts to syngas.

Table 1. The performance of catalysts in cellulose steam reforming.

Sample	H_2 production rate (mmol $g^{-1}_{catalyst}$ h^{-1})	CO production rate (mmol $g^{-1}_{catalyst}$ h^{-1})	Char yield (%)	Tar yield (%)	η value (%)
Ni-free Ce_3La_1	21.36	16.79	10.57	62.41	1.47
Ni/CeO_2	2389.7	782.2	3.4	69.3	3.6
Ni/Ce_5La_1	4059.6	1886.0	4.3	45.3	7.0
Ni/Ce_3La_1	4845.9	2778.5	3.1	26.9	7.6
Ni/Ce_1La_1	3646.7	2132.0	3.6	42.9	5.8
Ni/La_2O_3	2009.8	1289.4	3.6	64.9	3.3

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Acknowledgements: The authors thank National Natural Science Foundation of China (21972109, 21673168) for awarding the grant.

Yulu Zhang, a Master's student in Materials Science and Engineering at Wuhan University of Technology, China, focuses on photothermocatalytic cellulose steam reforming for syngas (H_2 and CO) production—a critical endeavor amid the global need for fossil fuel alternatives. She investigates Ni nanoparticle catalysts supported on La^{3+}-doped CeO_2 to boost syngas yields, reduce byproducts, and enhance light-to-fuel efficiency, while addressing the challenge of tar and char formation in biomass reforming. Her work contributes to the development of sustainable syngas production from renewable biomass resources.

EEPM5-CT-005

CONTRIBUTING TALK 5

Key Role of Light in Highly Efficient Photothermocatalytic Steam Cellulose Reforming on Ni-Based Catalyst

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KEYWORDS: Photothermocatalysis; Cellulose steam reforming; Green syngas

Photothermocatalytic cellulose steam reforming has emerged as a sustainable strategy for syngas (H_2 and CO) production from renewable biomass, offering a promising alternative to fossil fuel-dependent processes to advance carbon neutrality and circular sustainability. However, this approach is plagued by critical challenges: rapid catalyst deactivation due to excessive char and tar formation, low efficiency and limited solar utilization in photocatalysis, and inadequate syngas production rates, all impeding industrial application. To address these issues, a series of modified Ni nanoparticle-loaded catalysts have been developed. Ni-based catalysts exhibit remarkable performance, demonstrating significantly higher syngas yields and reaction efficiency in cellulose steam reforming compared to conventional catalysts. Herein, we find a photothermocatalyst of Ni nanoparticle-loaded θ-Al_2O_3 with an excellent capacity for consuming char in cellulose steam reforming under concentrated illumination. The catalysts achieve exceptional syngas production rates (H_2 3776.3, CO 2028.1 mmol $g^{-1}{}_{catalyst}$ h^{-1}) with excellent durability (e.g., no deactivation after 4 cycles) and reduced byproducts. With an emphasis on the mechanism, a different pathway is discovered that surface hydroxyl groups participating in the formation of HCO* intermediates, further dissociating to syngas, significantly facilitate the conversion ofchar. Notably, the role of light in the photothermocatalytic process is found to be multifaceted: beyond serving as a thermal source to maintain optimal reaction temperatures, it directly participates in activating Ni−O bonds on the catalyst surface, promoting the formation of H_2 and CO. In conclusion, through extensive experiments and characterization, we have elucidated the comprehensive mechanism of Ni/θ-Al_2O_3 catalysts in photothermal catalytic cellulose steam reforming reaction.

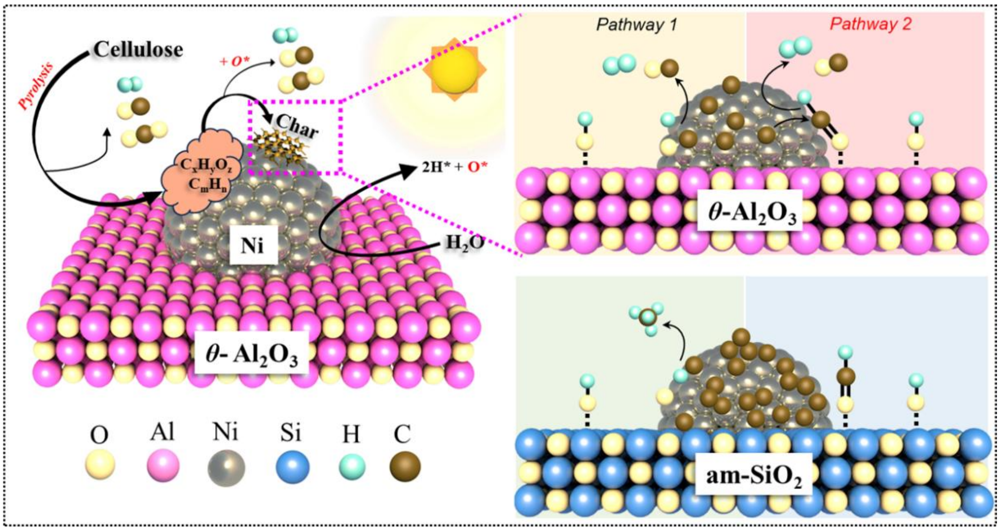

Figure 1. Schematically illustrative mechanism of cellulose steam reforming on Ni/θ-Al_2O_3 under concentrated illumination and two pathways of C* conversion over Ni/θ-Al_2O_3 and Ni/am-SiO_2.

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Acknowledgements: The authors thank National Natural Science Foundation of China (21972109, 21673168) for awarding the grant.

Jia Guo is a master's candidate at Wuhan University of Technology. Her research focuses on photothermal catalytic steam reforming of cellulose for syngas production—a green strategy to convert abundant biomass into valuable syngas using solar energy.

EEPM5-CT-006

CONTRIBUTING TALK 6

Deciphering Interfacial Kinetics in Nanostructured Oxide Semiconductors for Photoelectrochemical Water Oxidation Using Intensity-Modulated Photocurrent Spectroscopy

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KEYWORDS: IMPS; photoanode; photoelectrochemical water oxidation, charge carrier dynamics, oxide semiconductors.

The photoelectrochemical (PEC) production of green hydrogen presents a sustainable pathway for energy conversion by harnessing sunlight to directly drive water splitting reactions. This method offers a clean alternative to conventional hydrogen production by avoiding fossil fuel dependence. Despite its potential, achieving efficient and stable PEC performance remains a significant hurdle. Key parameters such as light harvesting, charge carrier separation, interfacial kinetics, and recombination processes need to be finely tuned. Advancing this technology toward practical applications requires a deep understanding of the involved materials and their interfacial behaviors.

To investigate the complex dynamics of charge carriers in PEC systems, intensity-modulated photocurrent spectroscopy (IMPS) was employed. By modulating the light intensity across a wide frequency range and analyzing the photocurrent response, this technique enables the deconvolution of overlapping processes like charge transfer, bulk and surface recombination, and electron–hole separation. These insights are crucial for identifying limiting steps and guiding the design of more efficient photoelectrodes [1].

In this work, we applied IMPS to study the charge dynamics in ternary copper vanadates and selected alloy compositions. Measurements were performed under varying experimental conditions as a function of applied potential, illumination wavelength, and light intensity, revealing trends in kinetic behavior. From these results, a kinetic model was established to describe how the hole transfer and surface recombination rate constants evolve in two boundary cases: one dominated by rapid recombination and another where recombination is minimal, as shown in Figure 1 [1].

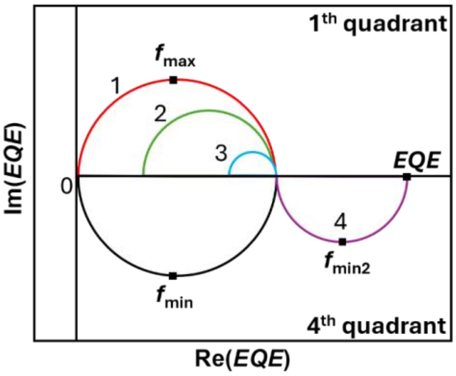

Figure 1. Schematic IMPS plot for different hole transfer (k_{tr}) and recombination (k_{rec}) rates. Case 1 for $k_{rec}>>k_{tr}$, case 2 for $k_{rec}=k_{tr}$, case 3 for $k_{rec}<k_{tr}$, and case 4 for $k_{rec}<<k_{tr}$.

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Acknowledgements: J.C. E-G. and G. O. gratefully acknowledge funding from Consejería de Universidad, Investigación e Innovación of the Junta de Andalucía (Spain) under grant ProyExcel_00543 (H2SOLDIR), the Ministerio de Ciencia e Innovación of Spain, Agencia Estatal de Investigación (AEI) and EU (FEDER) under grants TED2021-129758B-C33 (TransEL) and PID2022-140061OB-I00 (DEEPMATSOLAR). The authors also would like to thank for the support with characterization and materials analysis provided by INMALAB (Universidad Pablo de Olavide). A. R. and K. R. thank the National Science Foundation UTA/NU Partnership for Research and Education in Materials (DMR-2425164) for funding support.

Graduated in Environmental Sciences from Pablo de Olavide University (UPO) in Seville (Spain) in 2019, **Juan Carlos Expósito Gálvez** subsequently completed a Master's degree in Climate Change, Carbon and Water Resources at the same university in 2021. Since that year, he has been pursuing his PhD at UPO, focusing on the design of systems to improve the efficiency of solar photoelectrochemical water splitting based on metal oxides, with special emphasis on identifying the processes that limit system performance through advanced photoelectrochemical methods and theoretical modelling of electrical and electrochemical mechanisms. Currently, he is carrying out a research stay at the Faculty of Engineering, Department of Chemical Engineering, University of Malaya.

EEPM5-CT-007

CONTRIBUTING TALK 7

In-Situ Constructed Pt-Bi_2WO_6/g-C_3N_4 Heterojunction with Enhanced Charge Transfer for Dual Photocatalytic Applications

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KEYWORDS: Photocatalysis; Z-scheme; In-situ; Photocatalytic Water-Splitting; Electron Mediator

A high-performance Z-scheme photocatalyst, Pt-Bi_2WO_6/g-C_3N_4, was successfully synthesized via an in-situ hydrothermal method, where platinum (Pt) precursor was embedded into bismuth tungstate (Bi_2WO_6) during its partial formation using $NaBH_4$ as a reducing agent. This approach enabled the controlled reduction and incorporation of Pt into the monoclinic Bi_2WO_6 structure, followed by calcination with graphitic carbon nitride (g-C_3N_4) to form the final heterojunction. Compared to conventional photodeposition methods, the in-situ strategy provided significantly improved material dispersion, as evidenced by HRTEM images showing uniform Pt distribution and intimate contact between components. X-ray photoelectron spectroscopy (XPS) further confirmed the successful integration of Pt and enhanced charge flow, consistent with a Z-scheme mechanism facilitated by Pt as an electron mediator. Band structure analysis using Mott–Schottky plots and XPS revealed conduction and valence band edges at –0.43 eV and +2.17 eV, respectively, indicating a strong redox potential suitable for both dye degradation and hydrogen evolution. The optimized photocatalyst exhibited exceptional activity, achieving complete degradation (100%) of Rhodamine B dye within 45 minutes, with a rate constant of $0.1248\ \text{min}^{-1}$. In photocatalytic water splitting, the material generated 7.5 mL of hydrogen in 2.5 hours, corresponding to a solar-to-hydrogen (STH) efficiency of 58.81%. These results highlight the effectiveness of in-situ Pt embedding using $NaBH_4$ in constructing a robust Z-scheme system for sustainable environmental and energy applications.

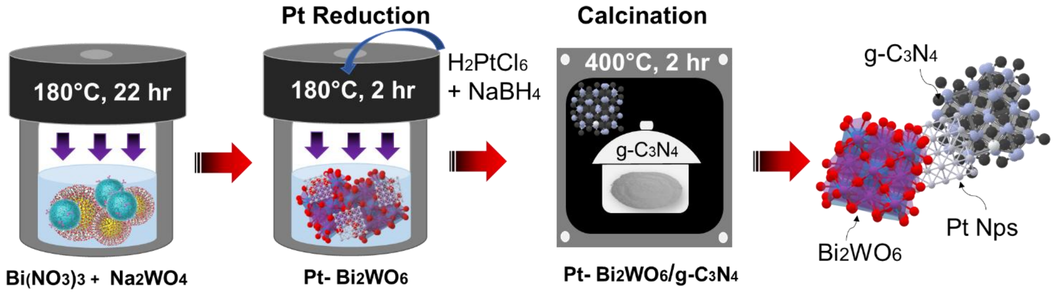

Figure 1. In-situ fabrication of Pt-Bi_2WO_6/g-C_3N_4

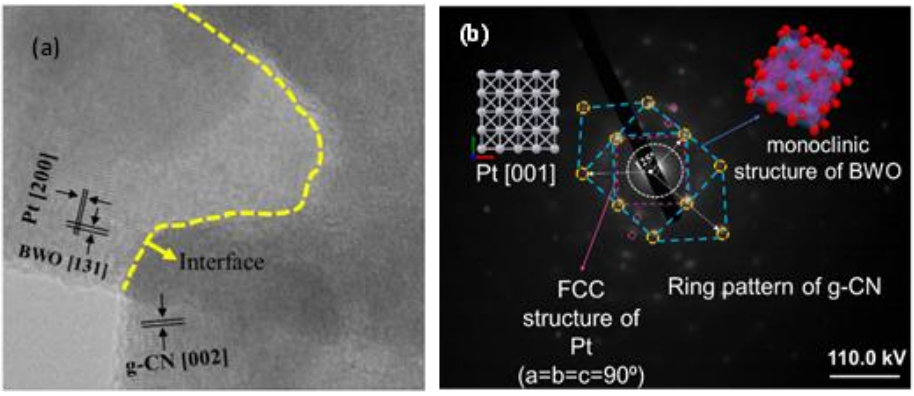

Figure 2: (a) High-resolution transmission electron microscopy (HRTEM) image, (b) Selected area electron diffraction (SAED) pattern of modified Pt-Bi_2WO_6/g-C_3N_4

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Acknowledgement: We would like to acknowledge Universiti Teknologi MARA (UiTM) and Universiti Teknologi PETRONAS for providing all the facilities for the completion of this research

Nur Syamimi Binti Mohamad Abdul Adzis is a Doctor of Philosophy (Science) candidate at Universiti Teknologi MARA (UiTM), Malaysia. Her research focuses on the development of Z-scheme heterojunction photocatalysts for solar-driven hydrogen production and wastewater remediation. She specializes in catalyst synthesis, semiconductor modification, and photoelectrochemical characterization. Nur Syamimi has published in high-impact journals such as ACS Omega and the International Journal of Hydrogen Energy, and her works have received numerous innovation and research awards. She has also been actively involved in international research collaborations with universities in China, Vietnam, and Jordan, contributing to the advancement of sustainable photocatalytic materials.

EEPM5-CT-008

CONTRIBUTING TALK 8

Optimizing IMS-MOF for Photo-Electrochemical Water Treatment via Band Gap Modification

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KEYWORDS: IMS-MOF; Photoelectrochemical degradation; Density Functional Theory (DFT); Band gap tuning; Methylene blue

This study reports the synthesis of a metal-organic framework-modified material (IMS-MOF), produced by modifying industrial iron metal sludge (IMS) with 1,3,5-benzenetricarboxylic acid (BTC) through a MOF-based approach. The material's efficacy was evaluated for the photo-electrochemical degradation of methylene blue (MB) under visible light irradiation. Density Functional Theory (DFT) simulations, performed using Material Studio, elucidated the structural, electronic, and adsorption properties of the synthesized IMS-MOF. Band gap analysis revealed a reduction from 3.54 eV for unmodified IMS, indicative of UV light absorption to 1.54 eV for IMS-MOF, thereby facilitating efficient photoactivation under visible light. This modulation of the optical response promoted enhanced charge carrier separation and consequently augmented light-assisted electrochemical degradation activity. Charge density mapping and adsorption behaviour simulations corroborated strong interfacial interactions between MB molecules and the active sites of the IMS-MOF, contributing to efficient pollutant degradation. A mechanistic pathway for the degradation process was proposed, integrating both theoretical modelling and experimental findings, underscoring the synergistic contributions of photoactivation, electrochemical reactions, and structural modifications induced by MOF incorporation. These results underscore the potential of IMS-MOF as a sustainable and high-performance material for the remediation of dye-contaminated wastewater.

Nurul Athikah Azizan is currently pursuing her PhD in the Faculty of Chemical Engineering at Universiti Teknologi MARA (UiTM), Malaysia. Her research focuses on transforming iron metal sludge (IMS), an industrial waste, into iron metal sludge–metal organic frameworks (IMS-MOF) using 1,3,5-benzenetricarboxylic acid (BTC) through MOF synthesis. By tailoring the band gap, her work enhances visible-light absorption for the photo-assisted degradation of methylene blue, contributing to sustainable wastewater treatment solutions. She obtained her Master's degree in environmental engineering, where she developed electrodes from IMS for the removal of methylene blue (MB), Reactive Black 5 (RB5), and Acid Blue 29 (AB29). Her research interests include photocatalysis, adsorption, and waste-derived materials for environmental remediation. She has published in both national and international journals.

EEPM5-CT-009

CONTRIBUTING TALK 9

PVDF/MoS$_2$/Fe$_2$O$_3$/GO Photocatalytic Membranes for Synchronous Cross-Flow Filtration and Photocatalysis

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KEYWORDS: Photocatalysis; Dye degradation; Visible-light; Cross-flow; Membrane

Integrating photocatalysis with membrane processes offers a promising pathway to mitigate irreversible fouling and enhance membrane longevity. In this study, we report a photocatalytic membrane reactor system constructed by coating a Molybdenum disulfide/ Iron oxide/ Graphene oxide (MoS$_2$/Fe$_2$O$_3$/GO) ternary Z-scheme composite photocatalyst on polyvinylidene fluoride (PVDF) ultrafiltration membranes. The photocatalyst was synthesized via a facile ball-milling and sonication method, followed by vacuum assembly of the composite on the PVDF membrane surface. The resulting membranes were evaluated in a cross-flow system (Fig.1) using Methylene Blue and Rhodamine B as model foulants, and characterized by structural and surface analyses including SEM, XRD, FTIR, AFM, contact angle and streaming potential. The composite-coated membranes exhibited enhanced membrane hydrophilicity, leading to reduced fouling and higher dye rejection. Under visible light irradiation, these membranes demonstrated a remarkable improvement in flux recovery and dye rejection compared to their performance in the dark. Specifically, 50 mg of photocatalyst coating increased the permeability for Rhodamine B from 13.46 kg/m^2/h in the dark to 52.99 kg/m^2/h under visible light and for Methylene Blue from 4.71 kg/m^2/h in the dark to 13.87 kg/m^2/h under visible light. The rejection values for Rhodamine B and Methylene Blue increased from 61.1% and 64.9% in the dark to 85.32% and 95.1% under visible light, respectively, after 180 minutes of filtration time. These performance enhancements are attributed to the synergistic effect of improved membrane hydrophilicity and Z-scheme charge separation within the photocatalyst, enhancing dye degradation. This study demonstrates that MoS$_2$/Fe$_2$O$_3$/GO photocatalyst coupled with PVDF membrane results in a bi-functional membrane, contributing to a more sustainable approach to wastewater treatment.

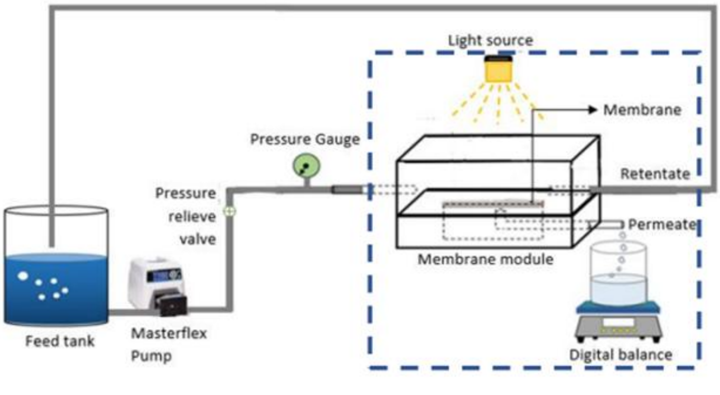

Figure 1. Experimental setup for cross-flow filtration and degradation studies.

L. Vishoda Samarasinghe is a PhD candidate in Engineering at Deakin University, Australia, supported by the Deakin University Postgraduate Research (DUPR) Scholarship. Her research focuses on developing photocatalytic membranes for wastewater treatment, with an emphasis on heterostructure photocatalysts and self-cleaning membrane technologies. She has presented her findings at international conferences and published in peer-reviewed journals in environmental nanotechnology and water remediation. Vishoda is a member of Engineers Australia (EA) and has prior experience in teaching and mentoring at the tertiary level. Her work aims to advance sustainable water treatment through the integration of photocatalysis and membrane-based processes.

EEPM5-CT-010

SPONSOR TALK

Integrated Multi-Technique XPS Approach for In-Depth Characterization of Energy and Environmental Photocatalysts

Hong Yuan Tok[1]

[1] Interscience Sdn. Bhd., 2, Jalan Sg. Kayu Ara 32/38, Berjaya Industrial Park, 40460 Shah Alam, Selangor, Malaysia.

This presentation highlights an integrated multi-technique XPS approach for in-depth surface and chemical characterization of photocatalysts. Through advanced depth profiling, high-resolution imaging, and multifunctional analysis, XPS provides detailed insights into elemental composition, oxidation states, and interfacial properties. Case studies illustrate how this method supports the development and optimization of efficient photocatalytic materials.

Mr. **Hong Yuan Tok**, Senior Application Specialist, Interscience Sdn. Bhd. with over 10 years of experience in SEM, TEM, FIB, AFM, Raman, and other analytical techniques. He supports researchers and industry partners in achieving high-quality results through advanced materials characterization.

POSTER PRESENTATION
BRIEF COMMUNICATIONS & SPEAKERS' PROFILES

List of Poster Presentation

Poster 1 **EEPM5-P-001** **Xuefei Wang**
Synchronous d-p Hybridization and Protonated State Regulation for Efficient H_2O_2 Photosynthesis through Optimized Water Oxidation

Poster 2 **EEPM5-P-002** **Xidong Zhang**
Directionally Modulating Free-Electron Transfer of MoS_x Cocatalyst for Improved Photocatalytic H_2O_2 Production

Poster 3 **EEPM5-P-003** **Ting Gao**
Highly Efficient H_2 Production over $NiCo_2O_4$ Decorated TiO_2 by Photocatalytic Water Splitting

Poster 4 **EEPM5-P-004** **Zhuonan Lei**
Stable and Efficient Photocatalytic H_2 Evolution over Twinned $Mn_{0.5}Cd_{0.5}S$ in NaOH Solution: Surface Reaction Kinetics and Energy-level Alignment Analysis

Poster 5 **EEPM5-P-005** **Wei Ping Wong**
Towards Universal Benchmarking of Photocatalysts Performance

Poster 6 **EEPM5-P-006** **Jun-Wei Khoo**
Maneuvering Deoxygenation Degree of Reduced Graphene Oxide (rGO) to Ameliorate Charge Mediation in Z-Scheme Photocatalyst for Methanol Photoreforming

Poster 7 **EEPM5-P-007** **Zak Jia-Xian Lee**
Synergistic Effects of CuSe-Decorated ZnO Photocatalysts for Efficient Hydrogen Evolution via Glycerol Photoreforming

Poster 8 **EEPM5-P-008** **Justin Khor**
Boosting CO_2 Photoreduction via Hollow and Size-Controlled Lead-Free

Poster 9 **EEPM5-P-009** **Wan Abdul Rashid W.E.S**
Round-The-Clock Photocatalysis for Sustainable Hydrogen Peroxide Generation

Poster 10 **EEPM5-P-010** **Inn Jynn Teh**
Unassisted Solar-Driven Water Splitting: $BiVO_4$ Photoanode for Sustainable Green Hydrogen Production

Poster 11 **EEPM5-P-011** **Eleen Dayana Mohamed Isa**
Photocatalytic Degradation of Simulated Textile Wastewater using Zinc Oxide-Polyaniline Nanocomposite

Poster 12 **EEPM5-P-012** **Jinfeng Zhang**
CeO_2 /$WO_{2.72}$ Nanocomposites with S-scheme Heterojunctions and Oxygen Vacancies for Enhanced Photocatalytic Degradation of Dichlorvos

Poster 13 **EEPM5-P-013** **Lin Zhang**
Visible-Light-Driven Metal-Free Photocatalysis for Biomass Valorization via Selective Lignin Bond Cleavage

Poster 14 EEPM5-P-014 Mušálek Ondrej
A Search for Optimal Exfoliation Conditions of Graphitic Carbon Nitride for Photocatalytic Degradation of Pollutants by Electrochemical Impedance Spectroscopy

Poster 15 EEPM5-P-015 Ting Zhang
Modification of Covalent Triazine Frameworks (CTFs) with Carbon Quantum Dots (CQDs) for Enhanced Photocatalytic Hydrogen Peroxide Production

Poster 16 EEPM5-P-016 Lili Xu
Dipole-Modulated Band Offset in the $CsPbBr_3$/Janus MSSe/$CsPbBr_3$ Heterotrilayers

Poster 17 EEPM5-P-017 Chee Yan Loh
Sustainable Ammonia Production Coupled with Biomass Upcycling via a Bifunctional MBene Electrocatalyst

EEPM5-P-001

POSTER PRESENTER 1

Synchronous d-p Hybridization and Protonated State Regulation for Efficient H_2O_2 Photosynthesis through Optimized Water Oxidation

Jing Zhang[1], Yu Wang[2], Qingzhe Zhang[1], Xuefei Wang[1], * Ping Wang[1], Feng Chen[1], Huogen Yu [3*]

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KEYWORDS: WOR; Fe–O–P d-p orbital hybridization; protonated state regulation; FeOOH/$BiVO_4$/Au; photocatalytic H_2O_2 production.

Photocatalytic H_2O_2 production is a promising sustainable approach due to safe operation, ambient reaction conditions, on-demand production, and availability of inexpensive raw materials. However, its practical application is hindered by inefficient interfacial catalytic activity, particularly in the WOR, which suffers from slow kinetics and low selectivity due to *OH intermediate adsorption weak and instability. To address these challenges, this study proposes a "Fe-O-P *d-p* hybrid orbital synergistic protonated state regulation" strategy to enhance WOR kinetics and selectivity for H_2O_2 formation. Specifically, FeOOH/$BiVO_4$/Au photocatalysts were synthesized via a two-step photodeposition method, integrating dual-cocatalyst modification to optimize active sites and suppress charge recombination. Subsequently, phosphoric acid impregnation was employed to construct $H_2PO_4^-$@FeOOH/$BiVO_4$/Au, where Fe-O-P *d-p* hybridization modulates *OH intermediate adsorption, while protonated state regulation enhances the selectivity of the two-electron WOR pathway. The optimized $H_2PO_4^-$@FeOOH(1.5%)/$BiVO_4$/Au(3%) catalyst achieved a remarkable H_2O_2 yield of 2321 μmol/L in 3 hours under pure water conditions, demonstrating a 6-fold enhancement compared to FeOOH/$BiVO_4$/Au.Notably, this catalyst exhibits the highest H_2O_2 production efficiency among the current bismuth-based photocatalytic material systems. The improved performance is attributed to (1) the construction of P-O-Fe *d-p* hybridization that elevate the Fe d-band center, enhancing *OH adsorption and facilitating electron transfer to accelerate WOR kinetics; and (2) the protonation effect of $H_2PO_4^-$, which stabilizes *OH intermediates and increases the selectivity of H_2O_2 formation over oxygen evolution. X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations confirm the role of Fe-O-P *d-p* hybridization in modulating the Fe d-band center and improving H_2O_2 selectivity. This study provides a new paradigm for the rational design of WOR-oriented photocatalysts and advances the field of photocatalytic H_2O_2 synthesis.

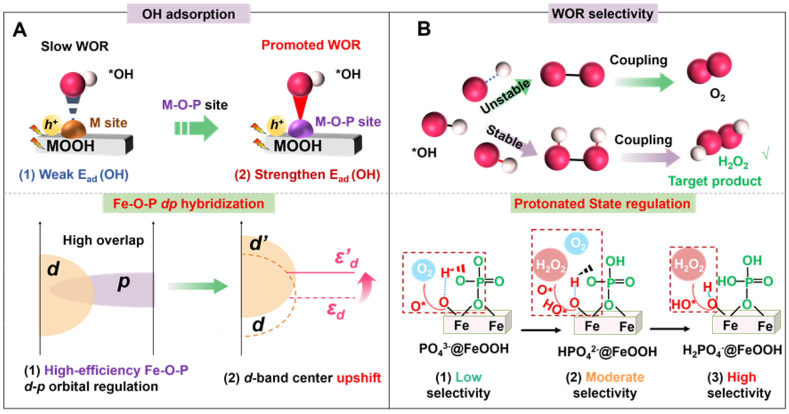

Figure 1. Illustrations of the basis for predicting how Fe-O-P *d-p* orbital hybridization in and protonation by the dihydrogen phosphate in $H_2PO_4^-$@FeOOH(1%)/$BiVO_4$/Au(3%) enhance the rate and selectivity of the WOR. (A) Schematic showing

how Fe-O-P site *d*-*p* orbital hybridization strengthens *OH adsorption via an increase of the d-band center leading to enhancement of the WOR (B) Protonation state regulation of *OH stability to improve two electron transfer and enhance formation of H_2O_2.

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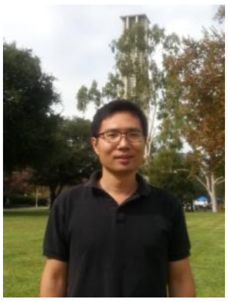
Acknowledgements: This work is supported by the National Natural Science Foundation of China (22178276, 22178275, U22A20147, and 22075220) and the Natural Science Foundation of Hubei Province of China (2022CFA001).

Dr. **Xuefei Wang** received his Ph. D. degree in materials science and engineering from the Wuhan University of Technology in 2011. He is now a professor at the School of Chemistry, Chemical Engineering and Life Sciences, Wuhan University of Technology. His research interest includes semiconductor photocatalysis, and functional nanomaterials.



EEPM5-P-002

POSTER PRESENTER 2

Directionally Modulating Free-Electron Transfer of MoS_x Cocatalyst for Improved Photocatalytic H_2O_2 Production

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KEYWORDS: Free electron transfer; O_2 adsorption; Cocatalyst; Photocatalytic H_2O_2 production

The electronic configuration mismatch between TiO_2 support and MoSx cocatalyst induces spontaneous free-electron transfer in an unfavorable direction, resulting in stronger O_2 adsorption on Mo active sites and causing limited H_2O_2 production. We propose a strategy of directional free-electron transfer to weaken O_2 adsorption on Mo sites for improving H_2O_2-production activity. To this end, we ingeniously constructed a core-shell Ag@MoS_x cocatalyst on the TiO_2 surface to synthesize the TiO_2/Ag@MoS_x photocatalyst. The resultant TiO_2/Ag@MoS_x photocatalyst achieves a significantly enhanced H_2O_2-production rate of 16.13 mmol g^{-1} h^{-1} with an AQY value of 8.79%. Theoretical calculations and experimental results reveal that the incorporation of Ag mediator in the TiO_2/Ag@MoS_x system can directionally facilitate free-electron transfer to the MoS_x cocatalyst. This results in increased antibonding-orbital occupancy of Mo-O_{ads}, ultimately weakening the Mo-O_{ads} bond and enabling high activity in H_2O_2 production. This study provides valuable insights into optimizing reactant adsorption for efficient artificial photosynthesis.

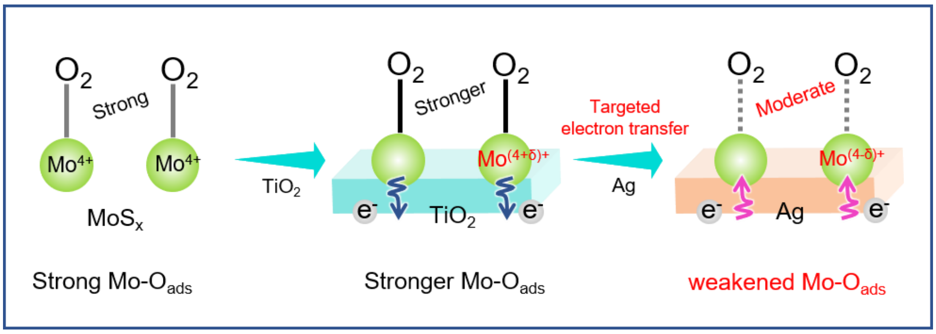

Figure 1. Schematic illustration of the free-electron directional transfer strategy to weaken Mo-O_{ads} bonds

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Dr. **Xidong Zhang** received his Ph.D. degree from Prof. Jiaguo Yu's research group at the China University of Geosciences (Wuhan). He is currently conducting postdoctoral research in Prof. Shaowen Cao's group at the Wuhan University of Technology. His research focuses on optimizing O_2 adsorption through cocatalyst design for photocatalytic H_2O_2 production.

EEPM5-P-003

POSTER PRESENTER 3

Highly Efficient H_2 Production over $NiCo_2O_4$ Decorated TiO_2 by Photocatalytic Water Splitting

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KEYWORDS: Photocatalytic H_2 evolution; $NiCo_2O_4/TiO_2$; S-scheme; Charge separation

Heterojunction engineering has been extensively demonstrated as an effective strategy to enhance the photocatalytic activity of single-component materials. In this work, a novel S-scheme $NiCo_2O_4/TiO_2$ heterojunction was successfully fabricated via a facile solvent evaporation method. The resultant composite exhibited markedly improved photocatalytic performance compared with pristine $NiCo_2O_4$ or TiO_2. Under the white light (full spectrum of the 300 W Xe lamp) irradiation, pure TiO_2 showed a hydrogen evolution rate (r_{H_2}) of 151.4 $\mu mol \cdot g^{-1} \cdot h^{-1}$ in 20 vol% triethanolamine (TEOA), which was constrained by rapid electron-hole recombination and a limited light absorption range. Notably, the optimized 15% $NiCo_2O_4/TiO_2$ composite achieved an exceptional r_{H_2} of 3507.6 $\mu mol \cdot g^{-1} \cdot h^{-1}$, representing a 23-fold enhancement over bare TiO_2. Furthermore, after three consecutive cycles, the composite retained approximately 85% of its initial activity. This could be associated with the consumption of the sacrificial agent. Combined XPS analysis and density functional theory (DFT) calculations revealed that the charge transfer between $NiCo_2O_4$ and TiO_2 follows an S-scheme mechanism, which not only facilitates spatial charge separation but also reduces the overpotential for H_2 evolution and extends light harvesting. This work provides a strategic design for high-efficiency TiO_2-based photocatalysts and advances the development of renewable H_2 energy.

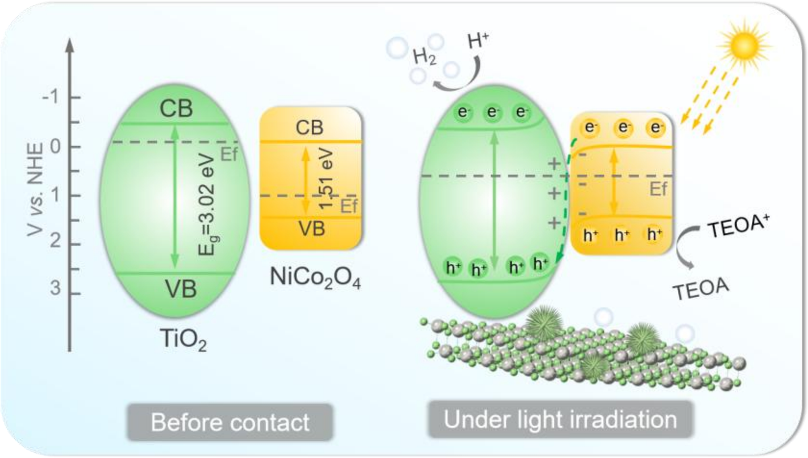

Figure 1. Schematic illustration of H_2 evolution over S-scheme $NiCo_2O_4/TiO_2$ heterojunction under light irradiation

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Acknowledgements: Thanks for the National Natural Science Foundation of China (No. 22378326, 22078261 and 11974276), Natural Science Basic Research Program of Shaanxi Province (No. 2023-JC-YB-115) and Shaanxi Key Science and Technology Innovation Team Project (2022TD-33) and Qin Chuangyuan project of Shaanxi Province (No. QCYRCXM-2022-213) for the financial support of this work.

Ting Gao earned her master's degree from the College of Chemical Engineering at Northwest University in 2017. As a core member of Prof. Enzhou Liu's research team, she focuses on synthesizing semiconductor photocatalytic materials for water splitting. With over 10 first - author or corresponding - author publications in renowned journals like International Journal of Hydrogen Energy and Journal of Alloys and Compounds, she has made significant contributions to the field.

EEPM5-P-004

POSTER PRESENTER 4

Stable and Efficient Photocatalytic H_2 Evolution over Twinned $Mn_{0.5}Cd_{0.5}S$ in NaOH Solution: Surface Reaction Kinetics and Energy-level Alignment Analysis

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KEYWORDS: Twinned $Mn_{0.5}Cd_{0.5}S$; Photocatalysis; Photocorrosion; Hydrogen evolution kinetics; Hydroxylated surface

Sulfides typically demonstrate exceptional efficiency as photocatalysts for hydrogen (H_2) evolution, but their practical application is constrained by rapid charge recombination, slow surface reaction kinetics and photocorrosion. In this study, we developed a hydroxide (OH^-) assisted strategy to overcome these challenges, using twinned $Mn_{0.5}Cd_{0.5}S$ (T-MCS) as a representative photocatalyst. We achieved stable and efficient photocatalytic H_2 evolution over T-MCS in NaOH solution without the need for any co-catalysts. The initial H_2 production rate over T-MCS at 308.15 K in 4 M NaOH can reach 21.04 $mmol \cdot g^{-1} \cdot h^{-1}$, which is 5.20 times higher than that in pure water. It was found that in alkaline solutions the surface metal hydroxylation can suppress the photo-corrosion of the S element and effectively enhance the stability of the catalyst. Moreover, the H_2 production activity of T-MCS exhibits a positive correlation with both the reaction temperature and the concentration of OH^-. Furthermore, according to the Langmuir-Hinshelwood kinetic model, energy-level alignment analysis and DFT calculations, the critical role of OH^- in accelerating the kinetics of the oxidation half-reaction was revealed. The investigation shows that the pathway for water oxidation shifts from a multi-electron reaction to a more kinetically favorable single-electron oxidation process in NaOH solution, thereby enhancing the driving force for OH^- oxidation and facilitating the formation of $\cdot OH$ radicals (Fig. 1a). And the detailed reaction equations over the photocatalytic water splitting in this highly alkaline environment reaction system are listed in Equations (1)-(4) below. During the HER, water molecules are decomposed into H_2 and OH^- by the photoexcited e^- generated by the catalyst. Simultaneously, the photogenerated h^+ oxidizes the introduced OH^- to generate $\cdot OH$, while a small quantity of free $\cdot OH$ radicals in solution may combine to generate H_2O_2 ($2 \cdot OH \rightarrow H_2O_2$). Trace amounts of H_2O_2 is detected in the liquid phase product with generation rates of 43.4 $\mu mol\ g^{-1} \cdot h^{-1}$ under the weakly alkaline environment. Furthermore, the consumed OH^- can be replenished through the dissociation of water, thereby promoting the continuous generation of H_2. It is evident that this represents a cascade reaction mechanism, which indicates that the theory of the consumption of OH^- does not affect the alkalinity of the solution to some extent. Additionally, the surface hydroxylation of T-MCS exhibits pH dependence (Fig. 1b), and the kinetics of the $\cdot OH$ formation process become increasingly favorable as the alkalinity of the solution increases.

$$H_2O \rightarrow OH^- + H^+ \qquad (1)$$

$$2H^+ + 2e^- \rightarrow H_2 \qquad (2)$$

$$OH^- + h^+ \rightarrow \cdot OH \qquad (3)$$

$$2 \cdot OH \rightarrow H_2O_2 \qquad (4)$$

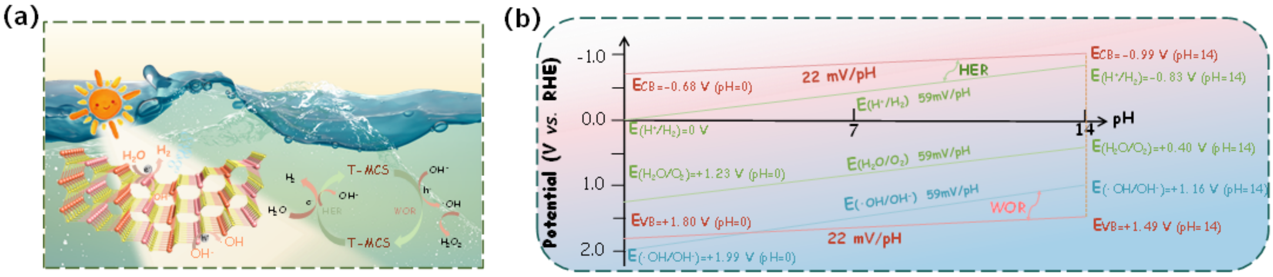

Figure 1. (a) The specific reaction process and (b) schematic energy-level alignment over T-MCS photocatalyst over this system

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Acknowledgements: This work was supported by the National Natural Science Foundation of China (22378326, 11974276, 22078261), Natural Science Basic Research Program of Shaanxi Province (2023-JC-YB-115), and Shaanxi Key Science and Technology Innovation Team Project (2022TD-33). Qin Chuangyuan project of Shaanxi Province (QCYRCXM-2022-213). Key Research and Development Program of Shaanxi Province (2024GX-YBXM-449).

Zhuonan Lei is a doctoral student at Northwest University, specializing in Chemical Engineering. Her main research focus is on renewable energy chemical engineering and biomass conversion, with a particular emphasis on photocatalytic water splitting for hydrogen production. This is a key direction in the development and application of solar fuels. Specifically, her work centers on constructing semiconductor-based photocatalytic systems: integrating the degradation of pollutants or the oxidation of cellulose into the water splitting process. The goal is to achieve efficient coupling of photocatalytic reactions, which is conducive to advancing sustainable energy conversion technologies. And as the first author, she has published 3 papers in top-tier SCI Q1 journals, including J. Mater. Sci. Technol., Chem. Eng. J. and Acta Phys.-Chim. Sin.

EEPM5-P-005

POSTER PRESENTER 5

Towards Universal Benchmarking of Photocatalysts Performance

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KEYWORDS: Photocatalysis; Quantum Efficiency; Apparent Quantum Efficiency; Standardized Performance Evaluation; Photon Flux Normalization

The progress of photocatalysis has long been hindered by the lack of a universal standard when comparing photocatalysts. This arises from the variations in reaction metrics, light intensity and spectrum, as well as reactor geometry [1]. As such, reported activities are not comparable across different laboratories despite testing the same photocatalyst and reaction. While common standards have been proposed over the years, they have not been popular since standardized setups can be costly (for example, those used in solar photovoltaic research), and information is not necessarily useful for further upscaling. At the same time, the use of chemical actinometry as a primary standard for normalization of activities is often cumbersome and with limited resolution on the “meaningful range” of photons [2, 3].

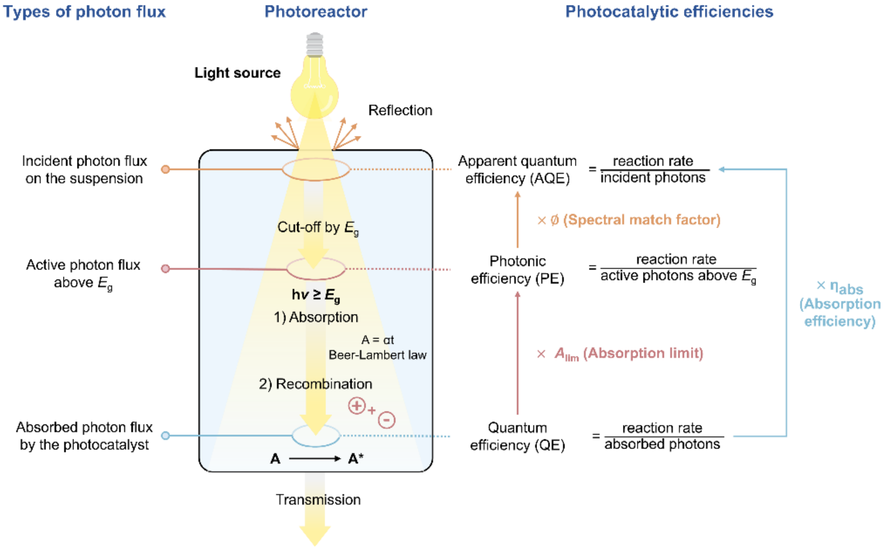

Figure 1. Schematic of photon transport in a photoreactor, illustrating reflection, absorption, recombination of charge carriers and transmission. The equations of AQE, PE, and QE are also shown.

Here, we introduce a unified framework that reduces the diverse literature-reported photocatalytic activity data into a single, consistent performance indicator, irrespective of light source or reactor configuration. The technique is based on photon counting as determined from the irradiation source with a defined spectrum and intensity [4]. When combined with the optical properties of the photocatalysts, this allows accurate quantification of apparent quantum efficiency (AQE), photonic efficiency (PE), and quantum efficiency (QE) (**Figure 1**). The relationship between these efficiencies allows elegant decoupling of the intrinsic activities of the photocatalysts from the reactor configurations and irradiation conditions. Our early demonstration of the technique enabled the rationalization of literature data on hydrogen evolution photocatalysts [5]. Here, we shall reveal for the first time the quantitative benchmarking of hydrogen evolution, oxygen evolution and organics degradation photocatalysts. The technique enables rigorous comparison of photocatalysts while preserving flexibility with regard to the experimental and reactor configurations under which they were evaluated. Without imposing a standardized setup, such robust benchmarking is crucial for aligning the communal efforts in photocatalyst development.

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Wei Ping Wong received her Bachelor's degree in Chemical Engineering from Universiti Malaya in 2022. She is currently a joint PhD candidate in Chemical Engineering at Universiti Malaya and the University of New South Wales (UNSW) Sydney, under the supervision of Scientia Prof. Rose Amal, Assoc. Prof. Wey Yang Teoh, and Dr. Denny Gunawan. Her research focuses on developing theoretical models to quantify photon flux and photocatalytic efficiencies, as well as upscaling photocatalytic reactor systems through multi-scale modelling.

EEPM5-P-006

POSTER PRESENTER 6

Maneuvering Deoxygenation Degree of Reduced Graphene Oxide (rGO) to Ameliorate Charge Mediation in Z-Scheme Photocatalyst for Methanol Photoreforming

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KEYWORDS: Photocatalysis; Photoreforming; Solar Hydrogen Harvesting; Z-Scheme; rGO

Methanol (CH_3OH) represents an ideal feedstock for photocatalytic hydrogen (H_2) production due to its high H:C ratio, low Gibbs free energy requirement, and potential to generate valuable formaldehyde (HCHO) as a liquid by-product. However, the rapid recombination of photogenerated charge carriers in pristine photocatalysts remains a critical bottleneck limiting photoreforming efficiency. To address this limitation, an all-solid-state Z-scheme photocatalyst with reduced graphene oxide (rGO) as charge mediator was developed. The impact of different reduction methods on graphene oxide (GO) was systematically investigated to optimize charge mediation performance. Three reduction approaches, thermal (Therm-rGO), chemical (Chem-rGO), and hydrothermal (Hydro-rGO), were employed to produce rGO variants with varying reduction degrees. Comprehensive characterization using XRD, FTIR, and Raman spectroscopy revealed that chemical reduction achieved the highest reduction efficiency, evidenced by minimal residual oxygen-functional groups and the highest I_D/I_G ratio in Chem-rGO. The enhanced structural defects and increased sp^2 clusters in Chem-rGO significantly improved charge percolation efficiency. When incorporated into a $ZnSe/Ag_2CO_3$ Z-scheme composite (Chem-ZGA), the Chem-rGO has enhanced optical absorption in the near-infrared region and dramatically improved charge migration and separation efficiency. This was confirmed by the lowest photoluminescence recombination rate, shortest average lifetime (τ_{ave}), and smallest Nyquist resistance arc observed for Chem-ZGA. The superior charge dynamics translated to exceptional photocatalytic performance, achieving H_2 and HCHO production rates of 88.6 and 264.7 $\mu mol\ g^{-1}\ h^{-1}$, respectively, during methanol photoreforming. These findings demonstrate that manipulating the reduction degree of rGO charge mediators in Z-scheme composites provides a viable strategy for optimizing photocatalytic performance in sustainable hydrogen production applications.

Acknowledgements: This work was supported by the Monash University Malaysia Future Centre for Net-Zero Technology (CNZT) under the Net-Zero Strategic Funding Scheme (NSFS).

Jun-Wei Khoo is a PhD candidate in the Chemical Engineering department at Monash University Malaysia, under the supervision of Dr. Siek-Ting Yong, Dr. Lling-Lling Tan, and Prof. Siang-Piao Chai. He has received his bachelor's degree with honours in Chemical Engineering from Monash University Malaysia in 2023. His doctoral research emphasizes on the application of Long Afterglow Phosphors (LAPs) for the development of Round-the-Clock (RTC) photocatalysts to facilitate diurnal hydrogen fuel production via ethanol photorefoming.

EEPM5-P-007

POSTER PRESENTER 7

Synergistic Effects of CuSe-Decorated ZnO Photocatalysts for Efficient Hydrogen Evolution via Glycerol Photoreforming

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KEYWORDS: Photocatalysis; Photoreforming; Advanced Functional Materials; Solar Hydrogen Harvesting; Renewable Energy

Glycerol photoreforming, an innovative and sustainable approach, has emerged as a promising technology for hydrogen production in recent years. This process harnesses solar energy to convert glycerol, a low-cost byproduct of biodiesel production, into hydrogen gas (H_2), a clean and versatile energy carrier as the main product. However, the widespread practical impact of this approach has been constrained by the modest efficiency of conventional photocatalysts, primarily due to their inadequate utilization of the solar spectrum. This report investigates the underlying mechanisms and key factors influencing glycerol photoreforming through the incorporation of copper selenide (CS) on zinc oxide (ZO). HRTEM, XRD and Raman analysis confirmed the successful synthesis of CS-loaded ZO (CSZO) samples. All CSZO samples exhibited broadened light absorption across the visible light range, based on UV-Vis analysis. TP and EIS analysis demonstrated that the combined presence of $Cu_{1.8}Se$, CS, and ZO propelled the kinetics of photogenerated charge-transfer and reduced interfacial resistance. These enhancements are attributed to the cooperative interfacial structure, in which the $Cu_{1.8}Se$ induces Rashba spin splitting and spin–momentum locking, thereby facilitating efficient carrier separation, and boosting mobility across the composite. Consequently, the augmentation of photogenerated charge carrier properties as well as the enhancement in light absorption capability elevated the H_2 production yield. A 50 wt% CS loading on ZO achieved an overall satisfying H_2 yield of 51.45$\mu mol \cdot g^{-1} \cdot h^{-1}$, representing a 1.76-fold enhancement compared to pristine ZO. Overall, glycerol photoreforming presents an exciting avenue for sustainable hydrogen production, accentuating the synergies between renewable energy utilization and waste valorization in the pursuit of a greener future.

Acknowledgements: This work was supported by the Monash University Malaysia Centre for Net-Zero Technology (CNZT) under Net-Zero Strategic Funding Scheme (NSFS).

Zak Jia-Xian Lee graduated with Honours in Chemical Engineering from Monash University Malaysia in 2022 and began his PhD in Chemical Engineering in 2023. His doctoral research focuses on photocatalysis, with a particular emphasis on glycerol photoreforming for hydrogen production. His work centers on catalyst development and mechanistic studies of charge transfer processes, aiming to advance fundamental understanding and improve efficiency in photocatalytic hydrogen generation.

EEPM5-P-008

POSTER PRESENTER 8

Boosting CO_2 Photoreduction via Hollow and Size-Controlled Lead-Free Perovskites

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KEYWORDS: Photocatalysis; Lead-free Perovskite; Morphology; CO_2 Reduction.

Photocatalytic carbon dioxide (CO_2) reduction offers a sustainable route to convert CO_2 into value-added fuels using solar energy. Among various photocatalysts, halide perovskite-based materials, specifically lead-based, have attracted significant attention for CO_2 reduction [1 2]. While lead-based halide perovskites have shown strong performance, their toxicity raises environmental concerns, highlighting the need for lead-free alternatives. In this study, we synthesized morphology-controlled $Cs_3Bi_2Br_9$ (CBB) photocatalysts via a simple antisolvent reprecipitation method under ambient conditions. Size reduction of CBB increased the density of active sites and suppressed charge recombination, enhancing photocatalytic efficiency. Furthermore, engineering a hollow structure (Figure 1 (a)) improved light harvesting, shortened charge transport pathways, and further promoted CO_2 adsorption (Figure 1 (b)). In addition, complementary computational analysis confirmed that vacancy formation in hollow structures facilitated charge redistribution and boosted CO_2 activation. Collectively, these structural modifications resulted in a 2.5-fold increase in methane (CH_4) production (2.66 $\mu mol \cdot g^{-1} \cdot h^{-1}$) for the optimized hollow, size-reduced CBB sample (CBB-MH). This work demonstrates a straightforward structural engineering strategy to advance lead-free perovskites as effective photocatalysts for CO_2 reduction.

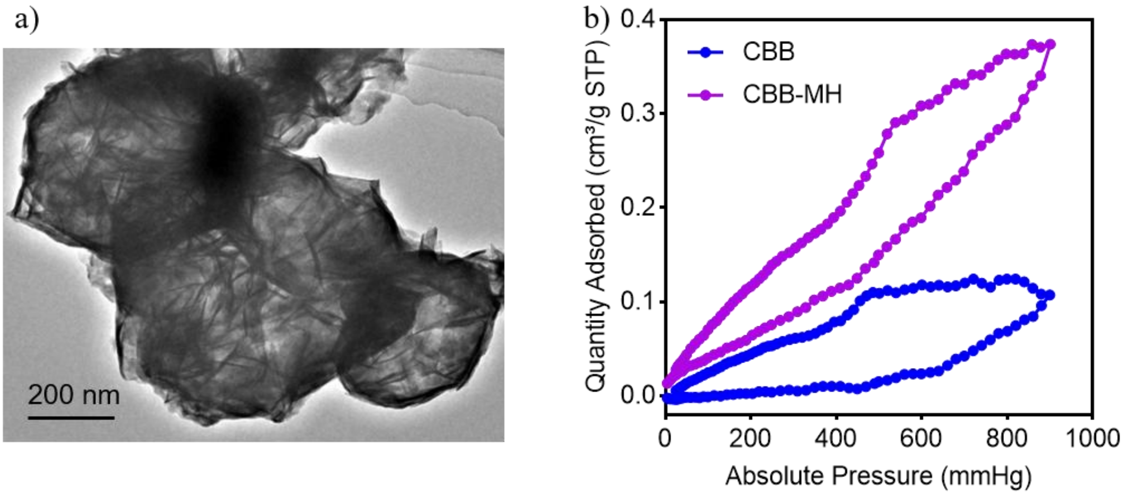

Figure 1. (a) TEM image of CBB-MH. (b) CO_2 adsorption of CBB-P and CBB-MH.

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Acknowledgement: This work was supported by the Monash University Malaysia Future Centre for Net-Zero Technology (CNZT) under the Net-Zero Strategic Funding Scheme (NSFS).

Justin Khor received his Bachelor of Chemical Engineering (Hons) from Monash University in 2023. He is currently pursuing his Ph.D. degree under the supervision of Dr. Lling-Lling Tan and Prof. Siang-Piao Chai. His research interests revolve around the design and development of perovskite-based materials for photocatalytic energy generation.

EEPM5-P-009

POSTER PRESENTER 9

Round-The-Clock Photocatalysis for Sustainable Hydrogen Peroxide Generation

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KEYWORDS: Photocatalysis; Round-the-clock Photocatalysis; Photochargeable Material; Hydrogen Peroxide

Hydrogen peroxide (H_2O_2) is a versatile oxidant with applications in wastewater treatment, disinfection, green chemical processes, and as a potential energy carrier [1]. However, conventional industrial synthesis, primarily through the anthraquinone process, is energy-intensive, centralized, and environmentally unsustainable [2, 3]. Photocatalytic H_2O_2 generation offers a greener approach by harnessing sunlight to drive oxygen reduction, yet conventional systems are limited by their reliance on continuous illumination [4, 5]. Photocatalysts based on graphitic carbon nitride (g-C_3N_4) have been extensively explored owing to their visible-light absorption, metal-free composition, chemical stability, and suitable band-edge positions for oxygen reduction [2, 3] Despite these advantages, pristine g-C_3N_4 is limited by rapid charge recombination and a negligible electron storage capacity, which hinders its ability to overcome the limitations of conventional photocatalysis [6]. To address these issues, we modified g-C_3N_4 into poly(heptazine imide) (PHI) through a molten-salt-assisted method, incorporating alkali ion intercalation and cyanamide functional groups. The resulting potassium-modified PHI (KPHI) was engineered as a photochargeable catalyst capable of sustaining “round-the-clock” photocatalysis, thereby enabling continuous H_2O_2 production under both light and dark conditions, as illustrated in Figure 1.

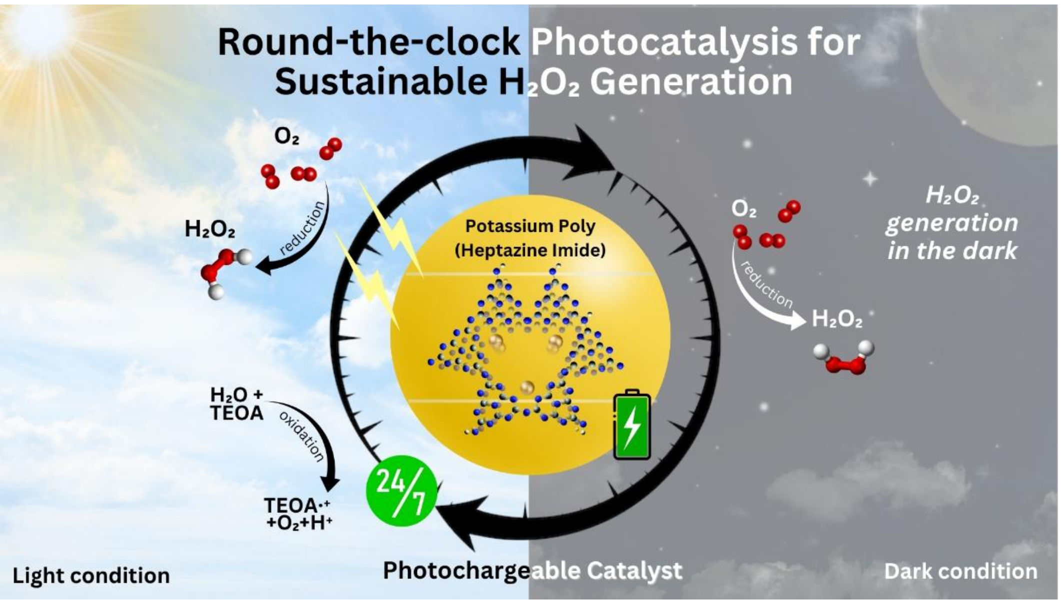

Figure 1. Day–night photocharge–discharge mechanism of KPHI enabling continuous H_2O_2 generation.

Comprehensive analyses were conducted using morphological (FESEM-EDX), optical (UV-Vis, PL), electronic (chronoamperometry, EIS), and charge storage (methyl viologen redox titration) techniques to assess its physicochemical, optical, and charge storage properties. Moreover, the photocatalytic H_2O_2 performance was evaluated under illumination and further monitored during subsequent dark periods. The modified KPHI photocatalyst exhibited enhanced visible-light absorption and suppressed PL intensity, confirming improved charge separation. Photoelectrochemical measurements revealed a higher photocurrent density and reduced charge transfer resistance compared to pristine g-C_3N_4. Importantly, charge storage evaluations demonstrated the ability of the alkali-modified framework to accumulate photogenerated electrons and act as an electron reservoir that can delay electron release. As a result, the photocatalyst sustained H_2O_2 generation even after illumination was switched off, with production increasing from ~6.0 µmol at 60 min (end of light period) to ~12.5 µmol at 100 min in the dark, before reaching a plateau and remaining stable. These findings demonstrate that structural engineering of g-C_3N_4, combined with alkali ion intercalation, effectively transforms a conventional photocatalyst into a photochargeable material with extended catalytic activity. This approach provides a new pathway for decentralized and sustainable H_2O_2 production, with potential scalability toward energy and environmental applications.

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Acknowledgements: This work was supported by the Centre for Research and Instrumentation Management (CRIM), Universiti Kebangsaan Malaysia.

Wan Emilin Suliza Wan Abdul Rashid obtained her BEng (Hons) in Chemical Engineering from Universiti Teknologi MARA (UiTM) and MEng in Electrical Engineering from Universiti Tenaga Nasional (UNITEN). She is currently pursuing a PhD in Chemistry at the Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia (UKM) under the supervision of ChM. Dr. Mohamad Azuwa Mohamed. Her research focuses on the design and modification of carbon nitride-based photocatalysts with charge storage capability to enable round-the-clock solar fuel generation through an artificial photosynthetic system.

EEPM5-P-010

POSTER PRESENTER 10

Unassisted Solar-Driven Water Splitting: $BiVO_4$ Photoanode for Sustainable Green Hydrogen Production

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KEYWORDS: Photoelectrochemical; Solar Hydrogen; Solar Fuel; Water Splitting; Bismuth Vanadate

The pressing need for a global clean energy transition in the upcoming years has sparked an unprecedent surge of interest in the development of green hydrogen production system. Hydrogen (H_2) has been acclaimed as the prime candidate of green fossil fuel alternatives as its combustion generates abundant energy and produces harmless water as the by-product. The photoelectrochemical (PEC) water splitting system has shown the brightest prospects for the commercialization of green hydrogen production, yet the kinetically limiting oxygen evolution reaction (OER) has stifled its potential. Therefore, there has been a surging interest in the development of a highly performing photoanode for the oxygen evolution reaction. Bismuth vanadate ($BiVO_4$) has shown boundless potential as a superior photoanode; however, its intrinsic limitation has constrained its practical application [1]. In this work, the construction of a self-driven solar water splitting system was successfully developed via the integration of a low-cost, commercial silicon solar cell with an earth-abundant $BiVO_4$ photoanode. A dual hole transporting layer of ferrihydrite and cobalt (oxy)hydroxide was incorporated onto $BiVO_4$ ($Co(O)OH/Fh/BiVO_4$) to improve and elevate the water oxidation performance of the photoanode in an overall water splitting system, leading to a 2.7-fold improvement in the photocurrent density at 1.23 V vs reversible hydrogen electrode (V_{RHE}) under AM 1.5 G irradiation [2]. The synergistic effects formed between the dual hole transporting layers with $BiVO_4$ has significantly averted the deleterious photogenerated charge carrier recombination, accelerated the water oxidation kinetics and enhanced the fill factor of the modified photoanode. A solar-to-hydrogen conversion efficiency (STH) of 1.38% was achieved for the self-assisted solar water splitting system, with a photostability of 24 hours. This work represents a pivotal advancement in the development of sustainable unassisted solar-driven water splitting system for solar fuels production.

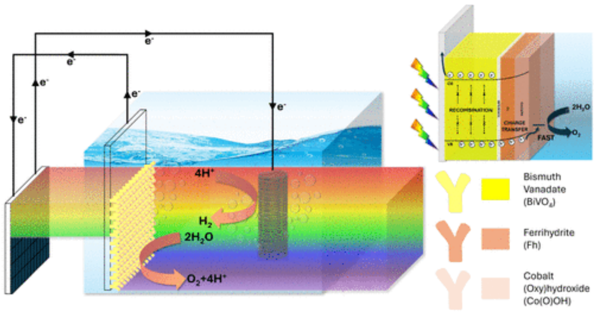

Figure 1. Unbiased solar-driven water splitting system with $Co(O)OH/Fh/BiVO_4$ as photoanode.

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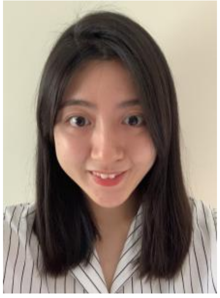
Acknowledgements: We gratefully acknowledge the funding support from PETRONAS Research Sdn. Bhd. (PRSB) through its Hydrogen Research Programme under the PETRONAS-Academia Collaboration Dialogue (PACD) 2022 (Project code: P-M010-CNI-000133), which supports the project and the PhD stipend of Inn Jynn Teh.

Inn Jynn Teh graduated with a Bachelor of Chemical Engineering (Honours) from Monash University Malaysia in 2022. She is presently pursuing her Ph.D. degree at the same institution under the supervision of Prof. Ir. Dr. Siang-Piao Chai, Prof. Ir. Dr. Meng Nan Chong and Dr. Lutfi Kurnianditia Putri. Her research is primarily focused on the development of solar-driven photoelectrochemical (PEC) water splitting system for sustainable green hydrogen production, alongside investigations into other value-added chemical conversion systems.



EEPM5-P-011

POSTER PRESENTER 11

Photocatalytic Degradation of Simulated Textile Wastewater using Zinc Oxide-Polyaniline Nanocomposite

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KEYWORDS: Photocatalysis; zinc oxide; polyaniline; simulated dye; mix dyes

Textiles are ubiquitous and essential to human life. As a daily necessity, the textile industry is a significant economic contributor in many countries. However, the textile manufacturing process, particularly dyeing, requires large volumes of water, leading to substantial wastewater generation. Unfortunately, this wastewater contains various classes of pollutants, with synthetic dyes making up a significant portion. In addition to altering the color of water bodies, these dyes are known to be carcinogenic, mutagenic, and highly toxic to all forms of life [1]. Among the various dye removal techniques, photocatalytic degradation stands out as a promising method. It utilizes light energy and a catalyst to break down pollutants, such as synthetic dyes [2]. The efficiency of this method is largely dependent on the type of catalyst used. In this study, zinc oxide–polyaniline nanocomposite (ZP NC) was synthesized and evaluated as photocatalyst for the degradation of simulated textile wastewater. Both zinc oxide (ZnO) and polyaniline (PANI) were synthesized in the presence of the biopolymer pullulan, which served as a capping agent. The nanocomposite was then fabricated using a chemisorption method. The synthesized catalyst was characterized using X-ray Diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR). The photocatalytic performance was tested using a simulated dye solution formulated by mixing five dyes: methylene blue (MB), crystal violet (CV), rhodamine B (RhB), methyl orange (MO), and methyl red (MR), each at a concentration of 10 ppm. The degradation experiment was carried out over three hours, during which complete discoloration was observed, and absorbance readings dropped to zero. Characterization results confirmed that the structural integrity of ZnO was retained after nanocomposite formation. FTIR analysis verified successful composite synthesis, indicated by characteristic bands representing both ZnO and PANI. Photocatalytic testing showed that the catalyst exhibited higher selectivity toward cationic dyes (RhB, CV, MB), which degraded more rapidly than anionic dyes (MO, MR). Despite this selectivity, the catalyst effectively degraded all dye types, demonstrating its strong potential for treating textile wastewater.

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Acknowledgements: The authors thank Universiti Teknologi Malaysia, UTMER 2024/1 (Q.K130000.3843.42J37) for supporting this research.

Dr. **Eleen Dayana Mohamed Isa** is a lecturer at Malaysia-Japan International Institute of Technology (MJIIT), Universiti Teknologi Malaysia Kuala Lumpur Campus. She is a newly hired staff and teach chemical engineering students the subject of analytical chemistry. In terms of research, she focusses on development of photocatalysts for degradation of pollutants. Throughout her years as research student to lecturer, she has produced several Web-of Science indexed research articles. Currently, she is also interested to venture towards catalyst development for electrocatalytic and photocatalytic reduction of carbon dioxide to useful chemical. Outside her professional life, she enjoyed playing badminton and discovering new cafes. Through this conference participation, she looks forward for opportunity to create new connections and learn other people research interest.

EEPM5-P-012

POSTER PRESENTER 12

CeO_2 /$WO_{2.72}$ Nanocomposites with S-scheme Heterojunctions and Oxygen Vacancies for Enhanced Photocatalytic Degradation of Dichlorvos

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KEYWORDS: Ultrafast Spectroscopy; Fs-TAS, Electron Dynamics; S-Scheme; Interfacial Electron Transfer

Confronted with escalating environmental challenges, photocatalytic degradation technology has become an effective solution for pollution control due to its efficiency, eco-friendliness, and sustainability. In this study, we synthesized CeO_2 /$WO_{2.72}$ nanocomposites (EO/WO) with S-scheme heterojunction structures and oxygen-rich vacancies and tested their ability to degrade the organophosphorus pesticide dichlorvos (DDVP) under visible light. The 30-EO/WO nanocomposite achieved an 89.9 % DDVP degradation rate in 80 min, significantly outperforming pure EO (67.5 %) and WO (64.7 %), and surpassing samples treated with a 5 h muffle furnace calcination. After four reuse cycles, the degradation efficiency of 30-EO/WO remained at 95.7 %, exceeding that of other control samples. This enhanced performance is attributed to the S-scheme heterojunctions and oxygen vacancies, which improve the separation of photogenerated electron–hole pairs, prevent their recombination, and extend carrier lifetimes, thereby boosting photocatalytic activity. Techniques such as electron paramagnetic resonance (EPR), surface work function measurements, and differential charge density calculations confirmed the formation of S-scheme heterojunctions and oxygen vacancies, elucidating the degradation mechanism. Simulated adsorption calculations showed that oxygen defect sites have a stronger adsorption capacity for DDVP molecules, enhancing reaction efficiency. Femtosecond transient absorption spectroscopy (fs-TAS) revealed that the synergistic interaction between S-scheme heterojunctions and oxygen vacancies plays a crucial role in improving photocatalytic performance.

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Acknowledgements: The authors thank the National Natural Science Foundation of China (42407636), the Major Foundation of the Educational Commission of Anhui Province (2022AH040068), the Anhui Province Discipline (specialty) Professional Leader Cultivation Project (DTR2024015).

Jinfeng Zhang: Professor and doctoral supervisor of Huaibei Normal University, provincial academic leader of Anhui Province. At present, His research mainly focuses on semiconductor nano photocatalytic materials and their applications in ecological environment and energy conversion. He has published more than 100 SCI papers in Nat. Commum., Appl. Catal. B: Environ., and other international academic journals, including 7 hot paper of ESI and 25 highly cited papers of ESI. It has been cited more than 9000 times, and the h-index is 55. It has mainly undertaken more than 10 research projects above provincial and ministerial level, including NSFC, China postdoctoral science foundation projects and Anhui major projects of Anhui Provincial Department of education.

EEPM5-P-013

POSTER PRESENTER 13

Visible-Light-Driven Metal-Free Photocatalysis for Biomass Valorization via Selective Lignin Bond Cleavage

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KEYWORDS: visible-light-driven conversion, lignin depolymerization, defect engineering, selective bond scission.

The transformation of lignin into renewable chemicals and energy carriers is a key challenge for achieving a sustainable bio-based economy. Traditional approaches such as thermal cracking or acid/base catalysis often require high energy demands and lead to environmental burdens. Recent advances in photocatalysis open new opportunities for low-carbon valorization strategies by utilizing visible light as a clean and renewable energy source.[1] In this context, we developed a metal-free organocatalyst that operates entirely without metals or corrosive additives.[2] The catalyst effectively promotes the scission of resistant interunit linkages in lignin under room temperature and atmospheric pressure, enabling selective depolymerization and conversion into value-added aromatic compounds. Beyond its catalytic efficiency, the system demonstrates stability and recyclability, which are crucial for long-term application. This study highlights a versatile platform for biomass utilization and illustrates how rational catalyst design can contribute to green chemical manufacturing, solar-driven fuel technologies, and the advancement of next-generation photocatalytic systems.

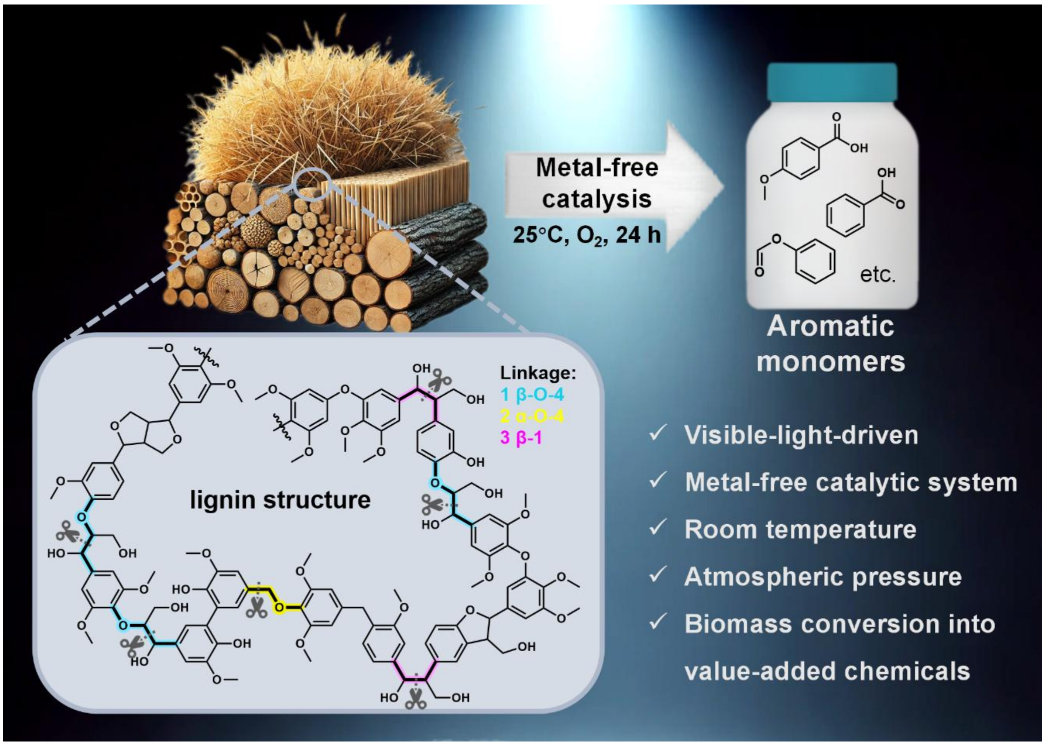

Figure 1. Metal-free photocatalytic valorization of lignin under ambient conditions

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Acknowledgements: T.P.L. gratefully acknowledges the financial support from the Distinguished University Professor grant (Nanyang Technological University), and the Agency for Science, Technology and Research (A*STAR) under its MTC Individual Research Grant (M21K2c0114) and RIE2025 MTC Programmatic Fund (M22K9b0049).

Ms. **Lin Zhang** is currently a Ph.D. candidate in the College of Advanced Interdisciplinary Science and Technology at Henan University of Technology. Her research is primarily devoted to photocatalytic biomass valorization, with a particular emphasis on lignin depolymerization for clean energy and useful chemicals production. She obtained her Master's degree in 2022 from Henan Institute of Science and Technology, where her work focused on biomass depolymerization for arabinose production. Ms. Zhang has authored in scientific publications in internationally recognized journals, including Materials Today Chemistry and Food Science and Technology. Her research aims to contribute to the development of sustainable photocatalytic strategies for addressing environmental issues.

EEPM5-P-014

POSTER PRESENTER 14

A Search for Optimal Exfoliation Conditions of Graphitic Carbon Nitride for Photocatalytic Degradation of Pollutants by Electrochemical Impedance Spectroscopy

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KEYWORDS: Photocatalysis; electrochemistry; nanomaterials

Environmentally friendly photocatalytic materials are increasingly sought after and one of the very promising ones is graphitic carbon nitride (GCN). High chemical and thermal stability, easy synthesis from abundant precursors and metal-free structure are some of its advantageous properties. However rapid charge carrier recombination, limited surface area, or relatively low quantum efficiency still hinder its practical application. [1] Thermal exfoliation is simple and cost-effective method to dramatically improve the photocatalytic properties of GCN. Mott-Schottky analysis and electrochemical impedance spectroscopy were used to investigate the electronic structure of exfoliated GCN. The conduction band potential was measured by Mott-Schottky measurement. Results from Mott-Schottky measurements suggest that exfoliation can be used to modify the conduction band potential and the band gap energy of GCN and potentially improve its photocatalytic properties. Electrochemical measurement in combination with photodegradation studies revealed an optimal degree of exfoliation for the best photocatalytic performance and provided deeper insight into the photocatalytic mechanism of action of these materials and will allow us to further improve their photocatalytic performance.

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Acknowledgements: This research was supported by the Czech Science Foundation under the project 24-10949S, by the Research Excellence for Region Sustainability and High-tech Industries project (REFRESH) (project no. CZ.10.03.01/00/22_003/0000048) and SGS project (SP2025/044).

Dr. **Mušálek Ondrej** completed his master's degree at University of Pardubice and is currently pursuing a Ph.D. at VSB-Technical University of Ostrava. His research focuses on exploring non-photocatalytic applications of graphitic carbon nitride, with an emphasis on its electrochemical properties and potential in energy storage systems. He has participated in several materials-oriented conferences across the Czech Republic, where he has presented and discussed advances in surface protection and energy conversion functional materials. His work aims to broaden the understanding of graphitic carbon nitride beyond its traditional photocatalytic domain.

EEPM5-P-015

POSTER PRESENTER 15

Modification of Covalent Triazine Frameworks (CTFs) with Carbon Quantum Dots (CQDs) for Enhanced Photocatalytic Hydrogen Peroxide Production

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KEYWORDS: Carbon Quantum Dots, Covalent Triazine Frameworks, Photocatalysis, Hydrogen Peroxide Production.

Harvesting renewable solar energy and harnessing Earth's abundant water resources to produce clean energy represents a pivotal strategy for achieving global carbon neutrality. Among various sustainable approaches, the solar-driven conversion of O_2 and H_2O into hydrogen peroxide (H_2O_2) using metal-free organic semiconductors with H_2O and O_2 as the sole feedstocks stands out for its inherent environmental benignity. As an ideal clean energy carrier, H_2O_2 yields only non-toxic H_2O and O_2 when decomposed catalytically for energy release or used as a fuel in fuel cells, with zero greenhouse gas emissions, thus realizing a "clean feedstock-to-clean product" closed loop. Herein, we report the development of a metal-free catalyst constructed by hybridizing carbon quantum dots (CQDs) with triazine-based covalent triazine frameworks (CTFs). CQD integration exerts a synergistic effect which enhances visible-light absorption, narrows the bandgap, and suppresses the recombination of photogenerated charge carriers, where all of which collectively boost H_2O_2 production. Our optimized CQD/CTF composite with 0.5 wt.% loading of CQDs achieves an exceptional H_2O_2 production rate of 2036.68 $\mu mol\ g^{-1}\ h^{-1}$ under visible light irradiation in pure water (without any sacrificial agents), which manifests 1.9 times higher than the pristine CTF and 271.6 times enhancement over the solitary CQDs. This work advances organic semiconductor design for efficient H_2O_2 synthesis from H_2O and O_2 in the absence of any sacrificial reagents, metals, or additives, offering a green and sustainable pathway to accelerate the global shift from fossil fuels to renewable energy carriers.

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Acknowledgements: T.P.L. sincerely acknowledges the financial support from the Distinguished University Professor grant provided by Nanyang Technological University, and the MTC Individual Research Grant (M21K2c0114) and RIE2025 MTC Programmatic Fund (M22K9b0049) provided by the Agency for Science, Technology and Research (A*STAR).

Ting Zhang is currently a Ph.D. candidate in the College of Advanced Interdisciplinary Science and Technology at Henan University of Technology. Her research primarily focuses on the effective utilization of solar energy to drive chemical reactions and to boost plant productivity. In 2020, Ms. Zhang earned her Master's degree from Zhengzhou University of Light Industry, where her work centered on water-soluble dietary fiber. She has published several academic papers in internationally renowned journals, such as Foods and International Journal of Biological Macromolecules. Ms. Zhang's work is committed to the efficient use of solar energy, both for enhancing plant yields and for producing solar-driven clean energy, thereby contributing to the advancement of agricultural sustainability and green energy development.

EEPM5-P-016

POSTER PRESENTER 16

Dipole-Modulated Band Offset in the $CsPbBr_3$/Janus MSSe/$CsPbBr_3$ Heterotrilayers

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***KEYWORDS**: Perovskite Solar Cells; Heterotrilayers; Nonadiabatic Molecular Dynamics; Band Offset; Density Functional Theory*

Perovskite solar cells (PSCs) exhibit remarkable photovoltaic efficiency, but energy level mismatches between the perovskite and charge transport layers often lead to severe nonradiative recombination, limiting device performance. To address this challenge, we propose a dipole-modulated heterotrilayer design by inserting two dimensional (2D) Janus MSSe (M = Mo, W) between $CsPbBr_3$ layers, forming a $CsPbBr_3$/Janus MSSe/$CsPbBr_3$ structure. The intrinsic dipole moment of the Janus interlayer generates a built-in electric field, which shifts the band edges of the adjacent $CsPbBr_3$ layers. This strategic modulation enables one $CsPbBr_3$ layer to function as the light absorber while the other acts as the hole transport layer, overcoming the limitations of conventional $CsPbBr_3$ homojunctions. Moreover, the band offset induced by the dipole effect depends on the dipole magnitude, which is too small to induce a significant band offset. Through nonadiabatic molecular dynamics simulations, we demonstrate that the WSSe-based heterotrilayer, with its stronger dipole moment and weaker nonadiabatic coupling, prolongs charge carrier lifetimes (4.343 ps) compared to the MoSSe-based structure (3.358 ps). This enhancement is attributed to suppressed carrier recombination and improved charge separation. Our findings highlight the potential of Janus-based heterotrilayers to enhance carrier separation and lifetime, offering a promising strategy to boost PSC efficiency.

Acknowledgements: We acknowledge the supports from the Singapore University of Technology and Design (SUTD) Kickstarter Initiatives (SKI 2021_04_01) and SMU-SUTD Joint Grant (22-SIS-SMU-054).

Lili Xu is a Ph.D. candidate in Materials Science and Engineering at Nanjing University of Science and Technology under the supervision of Prof. Shengli Zhang. Her research focuses on theoretical studies of carrier dynamics, perovskite optoelectronics, and computational catalysis using density functional theory and molecular dynamics simulations. She has published in high-impact journals such as *Nano Letters*, *Journal of Materials Chemistry A*, and *Applied Physics Reviews*. She previously earned her M.Sc. in Physical Chemistry from Jilin University and her B.Sc. in Environmental Analysis and Testing from Mudanjiang Normal University. Xu has been recognized with multiple academic awards, including Outstanding Graduate Student and an Excellent Poster Award at the 6th International Symposium on Advanced Inorganic Materials.

EEPM5-P-017

POSTER PRESENTER 17

Sustainable Ammonia Production Coupled with Biomass Upcycling via a Bifunctional MBene Electrocatalyst

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KEYWORDS: MBenes; Nitrate Reduction Reaction (NO_3RR); Glycerol Oxidation Reaction (GOR); Green Ammonia; Photovoltaic-Electrochemical (PV-EC) System

Ammonia (NH_3) is emerging as a promising hydrogen carrier for decarbonizing hard-to-abate sectors due to its high energy density and compatibility with existing distribution infrastructure. However, the conventional Haber-Bosch process remains energy- and carbon-intensive, necessitating greener alternatives [1]. Electrochemical NH_3 production via the nitrate reduction reaction (NO_3RR) offers a sustainable pathway that simultaneously addresses nitrate pollution—a prevalent anthropogenic pollutant in groundwater. Meanwhile, glycerol, an abundant byproduct of biodiesel production, can be upcycled through the glycerol oxidation reaction (GOR), providing a valuable feedstock for fine chemical production while replacing the sluggish and energy-intensive oxygen evolution reaction (OER). Herein, we report a bifunctional electrochemical system that integrates NO_3RR and GOR, enabled by FeB MBene electrocatalyst synthesized via a green, fluorine-free hydrothermal-assisted etching route from Fe_2AlB_2 precursors. The MBene features dual active sites: (i) metallic sites that facilitate water dissociation for proton (H^+) generation and (ii) boron sites that effectively activate nitrate species [2]. This tandem catalytic configuration promotes efficient proton-electron transfer while suppressing side reactions such as hydrogen evolution reaction (HER) and nitrogen (N_2) formation, leading to enhanced NH_3 selectivity and Faradaic efficiency (FE). The FeB catalyst achieved a maximum NH_3 Faradaic efficiency of 85.36% and an NH_3 yield of 10.41 mg h^{-1} cm^{-2} at -0.5 V vs. RHE. Furthermore, a self-powered photovoltaic-electrochemical (PV-EC) system coupling NO_3RR–GOR electrolysis with a silicon-based photovoltaic cell enabled unassisted, solar-driven green ammonia production with low energy consumption. This work demonstrates a scalable and energy-efficient strategy for sustainable ammonia synthesis, while simultaneously valorizing glycerol and remediating nitrate pollutants. The integrated platform offers a dual-benefit approach toward clean energy transitions and circular waste utilization.

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Acknowledgements: This work was funded by Xiamen University Malaysia under the Xiamen University Malaysia Research Fund (XMUMRF) (Ref. no.: XMUMRF/2024-C14/IENG/0071).

Chee Yan Loh is a Master’s candidate at Xiamen University Malaysia, specializing in green catalysis and sustainable energy solutions. Her research is centered on the development of advanced catalytic systems for sustainable ammonia production as a cleaner fuel alternative. During her undergraduate studies, she led a project on a barium oxide–reduced graphene oxide catalyst for biodiesel production, which demonstrated notable efficiency and reusability. In recognition of this work, she was awarded the 2023 POPSIG Student Research Project Bursary by the IChemE. Her current research focuses on ammonia production via nitrate reduction, integrating clean nitrogen-cycle technology with biomass valorization for sustainable energy innovation.

EEPM-5
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SPECIAL ISSUES

SPECIAL ISSUE 1

Chinese Journal of Catalysis

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Journal of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and the Chinese Chemical Society.

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SPECIAL ISSUE 2

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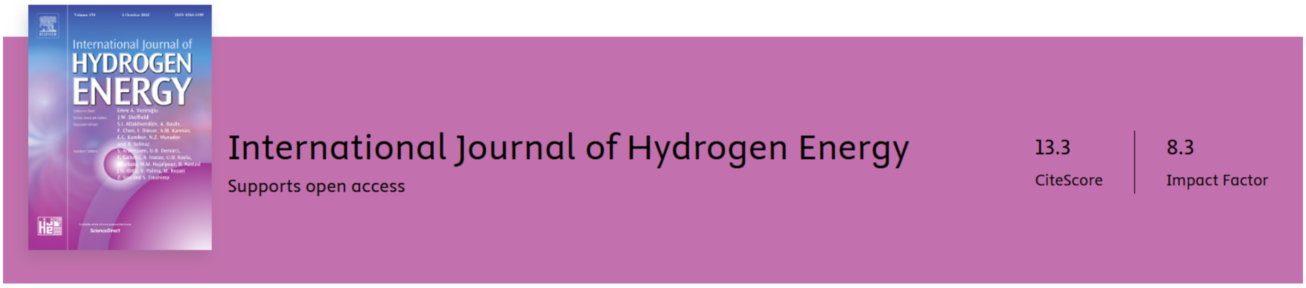

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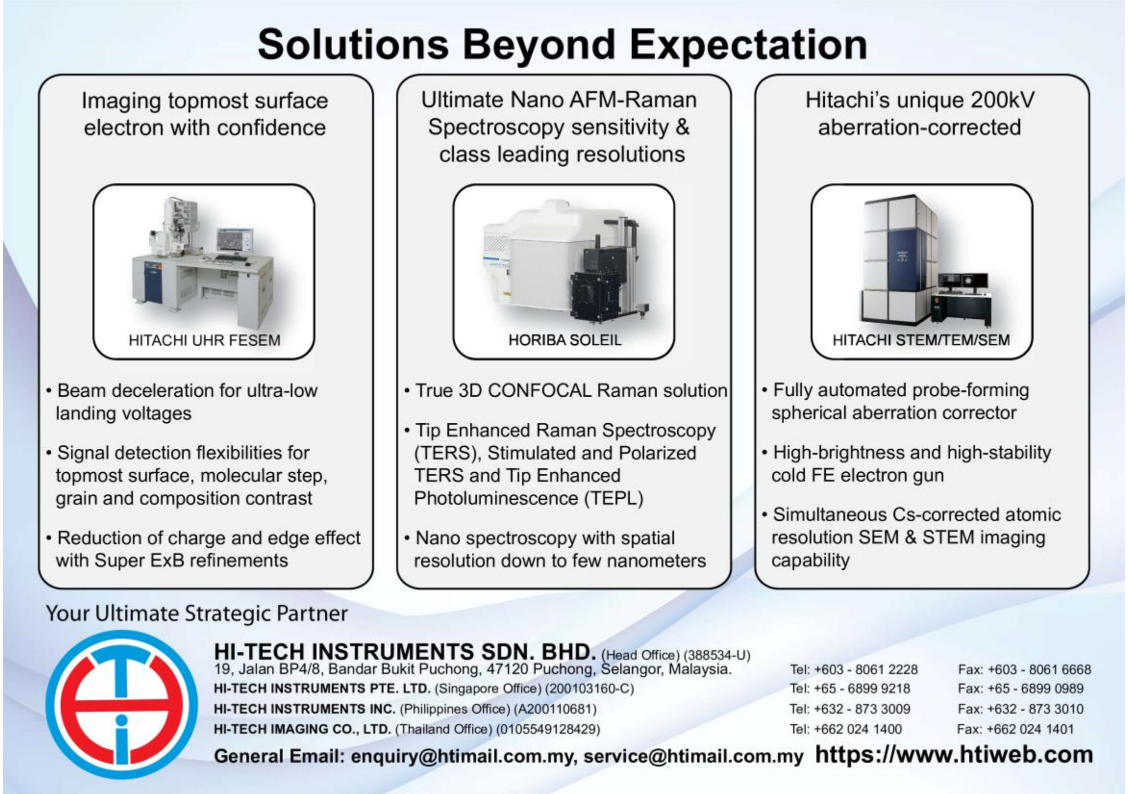

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