



BOOK OF ABSTRACT

9-10 SEPTEMBER 2024
HOTEL SERI MALAYSIA MELAKA

1ST INTERNATIONAL SYMPOSIUM ON SOLAR HYDROGEN 2024

Towards Green and Sustainable Hydrogen Future

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BOOK OF ABSTRACT

Institut Sel Fuel 2024

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INTRODUCTION



It is with great pleasure that we present the Book of Abstracts for the 1st International Symposium on Solar Hydrogen 2024, convened under the theme "Towards Green and Sustainable Hydrogen." This symposium represents a significant stride in our collective global pursuit of a sustainable energy future, with a specific focus on the advancement and refinement of solar hydrogen technologies. The gathering will unite preeminent experts, researchers, and practitioners from across the globe to disseminate their most recent discoveries and advancements in the realm of hydrogen energy. The symposium will address pivotal topics essential to the advancement of clean energy, including:

Solar and Photoelectrochemical Systems: Exploring the cutting-edge developments in solar-driven technologies for hydrogen production.

Sustainable Hydrogen Production, Storage, and Advanced Materials: Discussing innovative methods and materials for safe and sustainable hydrogen production.

Photocatalysis and Fuel Processing: Investigating the role of photocatalysis in enhancing the efficiency and sustainability of fuel processing.

Hydrogen Utilization, Safety, Technology & Others: Addressing the challenges and advancements in hydrogen storage, its practical applications, and the integration with battery technologies.

We aspire for this symposium to provide a platform for substantive discussions, knowledge exchange, and collaborations that will drive progress in the hydrogen economy. The contributions outlined in this Book of Abstracts signify the varied and dynamic research endeavors being undertaken in the pursuit of a more environmentally sustainable future.

We express our sincere gratitude to all the participants, contributors, and sponsors for their support in ensuring the success of this event. We are confident that the insights gained and the connections established during this symposium will serve as catalysts for further innovations and advancements in the field of solar hydrogen.

We appreciate your participation and valuable contributions to this significant discourse.

Sincerely,

Organizing Committee

1st International Symposium on Solar Hydrogen 2024

Plenary Presentation 1

OP-038 (P)

Solar Hydrogen: Current Status, Challenges, Opportunities and Future Direction for Green Hydrogen Production

Prof. Dato' ChM. Dr. Mohammad B. Kassim

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The work of Brattain and Garrett (Bell Telephone Laboratories) and Gerischer (Max Planck Institute, Stuttgart) defined the fundamentals for modern photoelectrochemistry. In fact, the terms photoelectrochemistry and photoelectrochemical cells that we use today originated from their publications. The study of photoelectrochemical cells attained tremendous interest after Fujishima and Honda and later, O'Regan and Grätzel published their work. The explosive interest may be associated with the energy crisis of the seventies when the World for the first time realised that the supply of fossil fuels cannot last forever and consequently, faces the climate change crisis due to the accumulation of greenhouse gases that originated from burning fossil fuels. The world needs to find a substitute that is clean and sustainable. Solar hydrogen emerges as a promising avenue for leveraging solar energy that in turn contributes to mitigating climate change and restricting fossil fuel combustion. This article focuses on photoelectrochemical (PEC) cells and accounts for the current development status, challenges and opportunities as well as future directions of PEC systems for sustainable hydrogen production. It presents different methods for converting abundant solar energy into hydrogen, and in turn, attaining the solar hydrogen fuel. The highlight on photoelectrochemical water splitting (PEC-WS) reveals the importance of PEC-WS for a green hydrogen production. Further discussion will emphasise the achievements of PEC-WS especially, in terms of materials used for the fabrication of photoanodes, photocathodes and tandem cells. The article also presents motivations for PEC-WS research in the near future specifically for green hydrogen contribution to the hydrogen economy. It is intended to be a manual for researchers new to the field and at the same time a useful reference for experienced researchers.



Biography

Mohammad B. Kassim, graduated with a B. Sc. (Hons.) in Chemistry with Energy & Fuel Science in 1992 from Lakehead University, Thunder Bay, Ontario, Canada and Master of Science (Chemistry) in 1996 from Universiti Kebangsaan Malaysia. He was conferred a PhD (Inorganic & Coordination Chemistry) by University of Bristol, United Kingdom in 2004. Currently, he serves as Professor of Inorganic Chemistry at the Department of Chemical Sciences, UKM. He was appointed as the Deputy Vice-Chancellor (Academic & International Affairs) from the 3rd of May 2021 to 2nd of May 2024. He was also appointed as the Chair for the Malaysia public university's Deputy Vice-Chancellor/Reactor for Academic Committee for (2024-2024). Previously, he served as the Dean for the Faculty of Science and Technology (2018 – 2021), Deputy Executive Director (Academic & Research) (2014 – 2017), Strategic Centre UKM. He has also been appointed as a Visiting Professor at University of Tsukuba (2019), Specially Appointed Professor at Osaka University (2018), Visiting Professor at Gifu University (2017), and Visiting Researcher at the University of Sheffield (2011). He specialised in coordination chemistry, molecular electronics, photoelectrochemistry, and conversion & utilization of CO₂. Currently, he is the founder and leader for Solar Hydrogen Research Group.

Plenary Presentation 2

OP-057 (P)

Ferrites in Energy Conversion Innovations: Breakthrough in Fuel Cells and PEC Water Splitting

Dr. Eng. Deni Shidqi Khaerudini

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For many years, ferrites, including iron oxalate, have been mentioned as one of the most important materials in widely used applications. This work endeavors to illuminate the applications of ferrites in energy conversion technologies, focusing in solid oxide fuel cells (SOFCs) and photoelectrochemical (PEC) water splitting. Iron oxalate, a precursor for iron-based nanomaterials, potentially reduces costs and increases efficiency. In SOFCs, ferrites enhance performance by improving conductivity and serving as electrocatalysts in solid ceramic cathode. In PEC water splitting, ferrites and iron oxalate (embedded with ZnO) function as photoanodes, improving sunlight absorption and facilitating efficient water splitting reactions for sustainable hydrogen generation. This study also explores future directions, highlighting research into environmentally friendly methods of synthesizing iron oxalate from steel industry waste. This not only leverages waste materials but also advances the application of ferrites in energy conversion technologies, combining environmental sustainability with technological progress. The potential of ferrites, especially iron oxalate, in revolutionizing energy systems is profound, pointing towards a greener and more efficient future.



Biography

Deni Shidqi Khaerudini, a Research Professor at the Research Centre for Advanced Materials, earned his PhD (Dr Eng.) from Hirosaki University, Japan, specializing in high-temperature fuel cell (SOFC) cathode materials. Following his graduation in 2016, he served as a Postdoctoral Fellow at the National Institute of Advanced Industrial Science and Technology (AIST), focusing on similar area of SOFCs cathode, specifically on nano manufacturing of vertically alignment cathode based on PLD. His research spans advanced material development for eco-friendly energy conversion, storage, low-carbon technologies, and management. He has authored over 200 papers in indexed journals, accumulating over 1012 citations and an h-index of 16.

Keynote Presentation 1

OP-055 (KN)

Potential of Atomic Layer Deposition in Improving Photoelectrochemical Water Splitting

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Efficient solar hydrogen (H₂) production, particularly using the photoelectrochemical (PEC) water splitting approach, faces significant challenges due to energy losses during light harvesting, recombination of photogenerated charge carriers, and electrode degradation. The stability and charge-transfer efficiency are critically dependent on the interfacial interactions between the electrode and electrolyte. Atomic Layer Deposition (ALD) is a key technology that addresses these challenges by enabling precise nanostructure development at the atomic scale. ALD facilitates bandgap engineering, surface passivation, catalyst improvement, and enhanced light-harvesting properties. In this talk, I will highlight ALD's pivotal role in improving the structural and surface properties of PEC electrodes and discuss their effects on PEC efficiency. Future research and innovation in ALD are essential for overcoming current limitations and achieving low-cost, large-scale, practical applications in sustainable hydrogen production.



Biography

Viet Huong Nguyen earned a B.S. in Materials Science from the National Institute of Applied Science of Lyon, France, in 2013, and a Ph.D. in Materials Science & Engineering from the University Grenoble Alpes, France, in 2018 (awarded the Best Ph.D. Thesis Prize by the French Chemical Society, Solid State Chemistry Division). Following this, he conducted postdoctoral research at the Laboratory of Materials Science and Physical Engineering (LMGP, CNRS) in Grenoble, France. Since August 2019, he has been a member of the Faculty of Materials Science and Engineering at Phenikaa University, where he currently serves as Vice Dean. His research focuses on the synthesis, surface engineering, and processing of nanostructured materials using Atomic Layer Deposition, with applications in flexible electronics, energy conversion, and storage.

Keynote Presentation 2

OP-048 (KN)

From Storage to Catalysis: The Versatility of Metal Hydrides in a Hydrogen Economy

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Hydrogen, a clean energy carrier, holds immense potential for decarbonization. However, storing hydrogen at high pressures (e.g., 700 bar) or cryogenic temperatures (-253°C) poses significant challenges for transportation and safety, particularly in remote areas. Metal hydrides offer a promising alternative by storing hydrogen in a solid-state form. This keynote will explore the fundamental principles of hydrogen storage in metal hydrides, discussing their advantages, limitations, and exceptional suitability for remote applications due to their high volumetric capacity and safe operation under practical conditions. To further enhance performance and address specific needs in remote areas, the use of composite materials will be discussed. Building on the understanding of metal hydrides as hydrogen storage materials, the presentation will explore their potential as catalysts in Liquid Organic Hydrogen Carriers (LOHCs). By examining how metal hydrides can accelerate hydrogen loading and unloading while addressing challenges such as high dehydrogenation temperatures and catalyst deactivation, their potential to improve LOHC efficiency will be explored. The presentation will conclude by emphasizing the crucial role of ongoing research in optimizing metal hydride performance to accelerate their widespread adoption in a hydrogen economy.



Biography

Kean Long Lim is a Senior Research Fellow and Associate Professor at the Fuel Cell Institute, Universiti Kebangsaan Malaysia (UKM). A registered Professional Technologist with the Malaysia Board of Technologists, Dr. Lim holds a Bachelor and Master of Chemical Engineering from UKM and a Ph.D. in Materials Science and Engineering from the University of New South Wales, Australia. His research focuses on electrocatalysts, hydrogen storage materials, fuel cell membranes, and renewable energy systems. He has led numerous research projects, published widely in international journals, and contributed to drafting technical codes for hydrogen storage in Malaysia. Dr. Lim has received several awards, including the MEXT Nuclear Researchers Exchange Program Fellowship from Japan and the UAiTED Faculty Exchange Scholarship from Taiwan. He has also been appointed as a Subject Matter Expert for the MyNet Zero Emission Roadmap 2050 by the Academy of Sciences Malaysia and served as an international grant evaluator for EPSRC in the UK. Dr. Lim's expertise in chemical engineering and materials science positions him as a key contributor to Malaysia's sustainable hydrogen economy transition.

Keynote Presentation 3

OP-056 (KN)

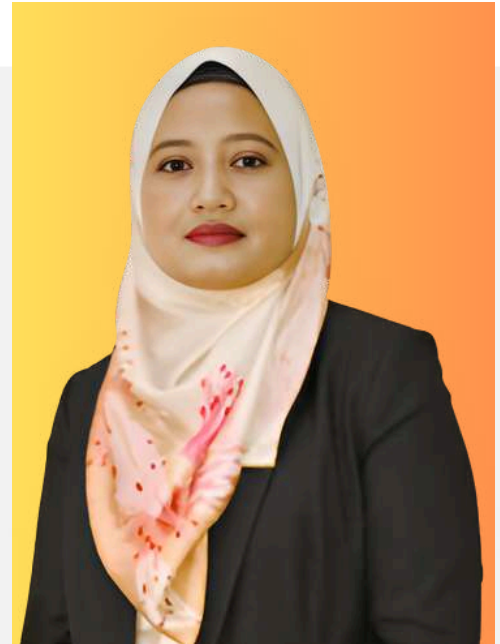
Research and Development of Hydrogen Energy Safety

Assoc. Prof. Dr. Rafiziana Md. Kasmani

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The increasing adoption of fuel cell vehicles (FCVs) and hydrogen refueling stations (HRSs) has heightened concerns about hydrogen leakage safety as recent fatal accidents underscore the potential risks of explosions, involving hydrogen jets and diffusion when hydrogen leaks from FCVs or HRSs. These accidents demonstrated intricate characteristics and posing significant technical challenges to make hydrogen powered vehicles as a game changer in transportation. Previous researchers have developed various theoretical models to understand the underlying mechanisms and introduced a range of monitoring and diagnostic approaches to detect and mitigate these hazards. This work delves into the safety implications of hydrogen leakage, examining different types of hydrogen jets, covering (1) subsonic jets, (2) underexpanded jets, their diffusion patterns in various environments, and strategies to mitigate hazards in both confined and open spaces. Additionally, it explores advanced hydrogen detection technologies. The ultimate goal is to identify research gaps and technological barriers hindering the development of robust safety standards, thereby facilitating the wider acceptance and utilization of hydrogen fuel cell technology in the transportation sector.



Biography

Rafiziana is a senior lecturer at the Department of Energy Engineering, Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia (UTM). Completed her PhD in 2009 at University of Leeds, UK, specializing in vented explosions. The main research focus is on fire engineering, gas and dust explosion by studying a series of methodologies for classifying flame acceleration and potential detonation hazard in chemical process industrial, including mixtures of different sensitivity. She managed to secure research grant with a total of more than RM2 million to date and published over 100 papers at the international and national levels in refereed journals and proceedings. For supervision, 5 PhD and more than 10 Masters has successfully graduated under her supervision with total current students of 2 PhD and 1 Masters. She also secured AUN-SEED Short-term Research Program in Japan (SRJP) JFY 2015 in University of Tokyo and a recipient of Fulbright Malaysian Scholar Program for 2017/2018 in University of Maryland, USA for six (6) month and selected as one of the recipients of Erasmus+ Mobility Staff Program in 2017 in Universidad Politécnica de Madrid (UPM). Through her experiences and expertise in Fire and Explosion engineering, Rafiziana has the opportunity to participate as a speaker in a variety of related courses, conferences and workshops and was invited as a keynote speaker at several international conference platforms.

Keynote Presentation 4

OP-054 (KN)

From Sunlight to Hydrogen: State-of-the-Art Advances in Photoelectrochemical Water Splitting for Sustainable Green Hydrogen Production

Prof. Ir. Dr. Chong Meng Nan

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Hydrogen, a clean energy carrier, holds immense potential for decarbonization. However, storing hydrogen at high pressures (e.g., 700 bar) or cryogenic temperatures (-253°C) poses significant challenges for transportation and safety, particularly in remote areas. Metal hydrides offer a promising alternative by storing hydrogen in a solid-state form. This keynote will explore the fundamental principles of hydrogen storage in metal hydrides, discussing their advantages, limitations, and exceptional suitability for remote applications due to their high volumetric capacity and safe operation under practical conditions. To further enhance performance and address specific needs in remote areas, the use of composite materials will be discussed. Building on the understanding of metal hydrides as hydrogen storage materials, the presentation will explore their potential as catalysts in Liquid Organic Hydrogen Carriers (LOHCs). By examining how metal hydrides can accelerate hydrogen loading and unloading while addressing challenges such as high dehydrogenation temperatures and catalyst deactivation, their potential to improve LOHC efficiency will be explored. The presentation will conclude by emphasizing the crucial role of ongoing research in optimizing metal hydride performance to accelerate their widespread adoption in a hydrogen economy.



Biography

Professor Ir. Dr. Chong has over 18 years of experience in academia, research, consultancy, and editorial work. His Ph.D. research, part of an ARC Linkage project, explored solar photocatalysis for reusing treated sewage effluents in South Australia. Before completing his Ph.D., he worked as a Research Scientist at CSIRO, leading urban water projects in Southeast Queensland. He later joined Monash University Malaysia (MUM), where he advanced from Senior Lecturer to Professor and now serves as Director of the Centre for Net-Zero Technology. He has secured over RM 20 million in research funding and received numerous awards, including the Royal Society of UK Newton Advanced Fellowship and recognition as a Top Research Scientist Malaysia. Ranked among the World's Top 2% Scientists by Stanford University from 2020 to 2023, Professor Chong is committed to fostering new research ideas and collaborations to drive innovation.

Invited Presentation 1

OP-020

Effect of Electrodeposited Cu₂O on Copper Foam Photoelectrodes for Enhanced Photoelectrochemical Water Splitting

Assoc. Prof. Dr. Lorna Jeffery Minggu

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Hydrogen is a promising alternative energy source to replace environmentally harmful fossil fuels. However, current hydrogen production methods lack efficiency and sustainability. This study explores the use of cuprous oxide (Cu₂O) electrodeposited on copper foam (CF) as a substrate to enhance the photoelectrochemical (PEC) water splitting process. Cu₂O layers were electrodeposited at -0.4 V for various durations (Cu₂O-x/CF where x = 5, 15, 30, 45, and 60 minutes). The structural, chemical and optical properties of the photoelectrodes were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and ultraviolet-visible spectroscopy (UV-Vis). XRD analysis confirmed the presence of Cu₂O, with diffraction peaks at 36.5° and 61.5° corresponding to (111) and (200) phases. SEM images showed well-spread Cu₂O particles on the photoelectrode, while UV-Vis spectroscopy indicated light absorption in the 350-600 nm range. Performance evaluation under dark and light using linear sweep voltammetry (LSV) showed photocurrent densities ranging from 1.23 to 3.33 mA/cm², with the Cu₂O-30/CF sample showing the highest photocurrent. Electrochemical impedance spectroscopy (EIS) results indicated the Cu₂O-30/CF sample has the least resistant. These findings suggest that Cu₂O electrodeposited on copper foam, particularly with a 30-minute deposition time, significantly enhances PEC performance, paving the way for the development of efficient, stable, and cost-effective Cu₂O-based photoelectrodes for sustainable hydrogen production.



Biography:

Lorna Jeffery Minggu (PhD) is an Associate Professor at Fuel Cell Institute, Universiti Kebangsaan Malaysia. She obtained her BEng in Chemical Engineering from UMIST, United Kingdom (now Manchester University), followed by her MSc and PhD in Chemical Engineering from Universiti Kebangsaan Malaysia. She is the head of the Photoelectrochemical Lab where she leads research in the development of advanced materials and systems for solar-driven photoelectrochemical (PEC) hydrogen production. Her research focused on the development of photoelectrocatalysts and photoelectrode materials for PEC water splitting, green hydrogen and solar fuels production, and also solar-driven environmental applications. Her research also includes the development of PEC cells and the integration of PEC system. She has successfully completed several projects that have resulted in various journal publications. She is also the coordinator and lecturer for the Hydrogen Energy course in MSc and PhD programs at the institute.

Invited Presentation 2

OP-018

Hydrogen Production Using 1D Modified TiO₂-Based Photocatalysts

Assoc. Prof. Ir. Ts. Dr. Lai Chin Wei

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Nowadays, serious environmental pollution and energy crisis are the most threatening problems to human kinds. Therefore, executing research for generating clean energy has been the passion for scientists, which can provide us energy in sustainable manner. In this manner, custom de-signed water splitter pumps out clean hydrogen gas for better hydrogen power performance is one of the most innovative solutions to supply recyclable hydrogen energy. The design and development of one dimensional (1D) WO₃- loaded TiO₂-based nanostructure film has gained significant interest in order to maximize specific surface area for harvesting more photons under solar energy. Based on our preliminary results, the incorporation of WO₃ into lattice of TiO₂ photocatalyst showed the promising performance. The coupling TiO₂ with small band-gap of WO₃ that possess different redox energy level for their valence band and conduction band, which provides another attractive approach to achieve more efficient charge separation under visible light. This condition will lead to additional electronic state in the band-gap, which in turn affect a change in the optical, electronic and functionality of TiO₂. It was found that the synthesized WO₃- loaded TiO₂-based nanostructure film demonstrated a maximum photocurrent density of ≈ 2.5 mA/cm² with photoconversion efficiency ≈ 6 %. The resultant photoelectrochemical performance was approximately two times higher than that of pure TiO₂ nanotubes film under solar illumination. The mediator of W⁶⁺ species will assist in trapping the photo-induced electrons and minimize the recombination of charge carriers during water electrolysis process.



Biography

Dr. Lai [PhD, BEng(Hons) | PEng, PTech, CEng (UK), MIEM, MIMechE (UK)] is currently an associate professor in Nanotechnology & Catalysis Research Centre, University of Malaya. Lai's main research interests are in the areas of chemically modified metal oxide photocatalysts, functionalized nanomaterials/nanocomposite and carbon graphene materials, especially apply in environmental pollution management and energy storage technology. As a scholar and an indication of the global impact of research work, Lai's works have been published in more than 300 refereed international top-tier journals with Scopus h-index of 45, 100 book chapters, and 100 international proceedings in materials science, physics, chemistry, and renewable energy researches. Through his work nanomaterials and catalysis field, Lai was awarded as APEC Science Prize for Innovation, Research and Education (ASPIRE) 2023 National Winner, IMechE Best Young Member Award 2022, JCI TOYM - Ten Outstanding Young Malaysians 2021 (Academic Leadership and Accomplishment), National Young Scientist Award 2019 by The Ministry of Energy, Science, Technology, Environment and Climate Change (MESTECC), MASS Young Researcher Award 2018 by Malaysian Solid State Science & Technology Society (MASS), a finalist of National Young Scientist Award 2018 by Ministry of Science, Technology and Innovation of Malaysia (MOSTI) and University of Malaya Excellence Awards 2015 in the category of outstanding researcher - UM Young Researcher (Sciences Discipline).

Invited Presentation 3

OP-040

Exploring Bismuth Ferrite Nanostructures for Effective Photocatalytic and Adsorptive Dye Degradation

Assoc. Prof. Dr. Siti Fairus Mohd Yusoff

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This study investigates the use of bismuth ferrite (BFO) nanostructures synthesized and intercalated within a liquid natural rubber (LNR)-acrylic acid (AAc) hydrogel matrix for the removal of cationic dye effluents from wastewater. By optimizing synthesis and degradation parameters using Response Surface Methodology (RSM), we achieved a highly efficient hydrogel-based photocatalyst that obviates the need for post-treatment separation. The hydrogel demonstrated remarkable stability, maintaining up to 99% dye removal efficiency over six cycles for safranin and five cycles for MB. Under xenon lamp irradiation, the rapid adsorption and photodegradation of MB and safranin dyes highlighted the significant photocatalytic capabilities of BFO nanostructures. The formation of reactive oxygen species, specifically hydroxyl radicals ($\cdot\text{OH}$) and superoxide radicals ($\cdot\text{O}_2^-$), was confirmed as the primary mechanism underlying the enhanced photocatalytic activity. The adsorption process adhered to a pseudo-second-order kinetic model and a Freundlich isotherm, indicative of the surface heterogeneity and multilayer adsorption on BFO. Thermodynamic analyses revealed a positive entropy change (ΔS), suggesting increased randomness and spontaneity in the adsorption process. Furthermore, the adsorption rate of safranin showed a strong dependence on pH, governed by inner sphere surface complexation, a key aspect of inorganic chemistry. Our findings underscore the potential of LNR-g-MaH/AAc-BFO hydrogel composites in advanced wastewater treatment, leveraging the robust photocatalytic and adsorptive properties of BFO nanostructures. This research contributes to the field of inorganic materials by demonstrating the effective application of BFO in environmental remediation, paving the way for the development of more efficient and sustainable inorganic photocatalytic systems.



Biography

Siti Fairus received a Bachelor of Science (Pure Chemistry) from Universiti Teknologi Malaysia (2007) and a Doctor of Philosophy in the same field from the University of Bristol in the United Kingdom (2011). Currently, she is a senior lecturer at Faculty of Science and Technology, Universiti Kebangsaan Malaysia. Her research focuses on the development of polymer and inorganic materials for different applications, such as wastewater treatment, agriculture, and biomedicine.

Invited Presentation 4

OP-039

Inorganic Modulation of g-C₃N₄ Photocatalysts for Enhanced Solar Fuel Generation

ChM. Dr. Mohamad Azuwa Mohamed

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Graphitic carbon nitride (g-C₃N₄) has emerged as a promising photocatalyst for solar fuel generation due to its unique electronic structure, thermal stability, and earth-abundant nature. However, its practical application is limited by inherent constraints, such as a moderate band gap, rapid recombination of photogenerated electron-hole pairs, and insufficient absorption of visible light. However, its practical application is limited by inherent constraints, such as a moderate band gap, rapid recombination of photogenerated electron-hole pairs, and insufficient absorption of visible light. In order to tackle these challenges, researchers have explored different inorganic modulation strategies to improve the photocatalytic performance of g-C₃N₄. A commonly used method is elemental doping, which involves adding metal and non-metal elements to adjust the band gap, widen the light absorption range, and improve charge separation efficiency. For example, metal dopants such as iron and cobalt, and non-metal dopants like phosphorus and sulfur, have been demonstrated to greatly enhance the photocatalytic activity of g-C₃N₄. The formation of heterojunctions with other semiconductors, such as TiO₂, WO₃, and ZnO, has been effective in facilitating efficient charge transfer and separation. This boosts the photocatalytic performance. Another promising strategy is the development of S-scheme heterojunctions, which combine the advantages of both conventional type-II and Z-scheme systems. This approach improves the redox ability and ensures strong oxidative and reductive power. The careful design of these heterojunctions results in a built-in electric field that promotes charge separation and minimizes recombination. The combined use of these inorganic modulation techniques advances the potential of g-C₃N₄ as a highly efficient photocatalyst for solar-driven water splitting, CO₂ reduction, and pollutant degradation.



Biography

Mohamad Azuwa Mohamed is a Senior Lecturer at the Department of Chemical Sciences, Faculty of Science and Technology, UKM. He received his Bachelor of Science (Industrial Chemistry) and Master of Engineering (Gas) degree from Universiti Teknologi Malaysia (UTM) in 2010 and 2015. In 2019, he obtained his Ph.D in Hydrogen Energy from UKM. He stands at the forefront of cutting-edge research on the intersection of photocatalysis, renewable energy, and environmental chemistry, addressing critical contemporary issues, by making substantial contributions that have garnered international acclaims. He gained recognition as the *World Top 2% Scientists* by Elsevier BV and Stanford University for four consecutive years starting from 2019 to 2022. He has pioneered the development of bio-templated 3D porous microtubular C-doped g-C₃N₄, and has set the trend to revolutionise the field of photocatalysis. In 2018, he received the Australian government's prestigious award under the *Endeavour Australia Cheung Kong Research Fellowship* at the University of New South Wales, Sydney, Australia. In 2019 and 2023, he was one of the *UKM Bitara Awards (Articles in Journal)* and *UKM Excellent Service Award* recipients. In 2023, he received a prestigious *Malaysia Young Scientist Award 2023 (Physical Science)* from the Ministry of Science, Technology, & Innovations (MOSTI) as recognition of his excellence in scientific research & development.

Invited Presentation 5

OP-030

Formic Acid Decomposition into Hydrogen Using Graphitic Carbon Nitride Supported Palladium Catalyst

Dr. Khairul Naim Ahmad

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Hydrogen production through the decomposition of formic acid (HCOOH) presents a promising alternative to reduce fossil fuel dependence and mitigate global warming. Formic acid is an efficient hydrogen carrier for hydrogen gas generation and storage. Palladium (Pd) is identified as a suitable catalyst for this process due to its ability to produce substantial hydrogen amounts during formic acid decomposition. However, challenges such as the deactivation of active Pd metal due to the formation of passive layers (e.g., formate compounds) and particle agglomeration at high Pd loadings need to be addressed. This study investigates the production of Pd catalysts with varying metal loadings (5–15 wt.%) using graphitic carbon nitride (g-C₃N₄) as a support material. Graphitic carbon nitride is synthesized via a thermal condensation method, and the Pd-supported g-C₃N₄ (Pd/g-C₃N₄) catalysts are prepared through impregnation technique. Morphological analysis confirms the successful dispersion of Pd particles on g-C₃N₄, forming small crystals. Crystal size analysis reveals that the intensity of peaks related to g-C₃N₄ decreases with increasing Pd loadings (5 to 15 wt.%), indicating that Pd inhibits the growth of g-C₃N₄ crystals. The performance of Pd/ g-C₃N₄ catalysts is evaluated for formic acid decomposition to produce gas. At 30 °C and 90% formic acid concentration, the 15 wt.% Pd/g-C₃N₄ catalyst achieves the highest gas volume of 38 mL in one hour, compared to 27 mL and 20 mL for the 10 wt.% and 5 wt.% Pd/g-C₃N₄ catalysts, respectively. However, at 75°C, all catalysts exhibit particle agglomeration, reducing their catalytic activity. High catalytic activity is maintained at 30°C. These results demonstrate that the 15 wt.% Pd/g-C₃N₄ catalyst outperforms the 5 wt.% and 10 wt.% Pd/g-C₃N₄ catalysts in terms of gas production volume, suggesting its potential for efficient hydrogen production through formic acid decomposition.



Biography

Dr. Khairul Naim Ahmad is a lecturer in the Department of Chemical & Process Engineering at Universiti Kebangsaan Malaysia (UKM). He holds a PhD in Chemical Engineering from UKM, where he also earned his Master's degree in Chemical Engineering. Dr. Khairul Naim completed his Bachelor's degree in Chemical Engineering at the Polytechnic University of Catalonia in Spain. His research primarily focuses on heterogeneous catalysis, process simulation, and CO₂ valorization, contributing to advancements in these critical areas of chemical engineering.

Invited Presentation 6

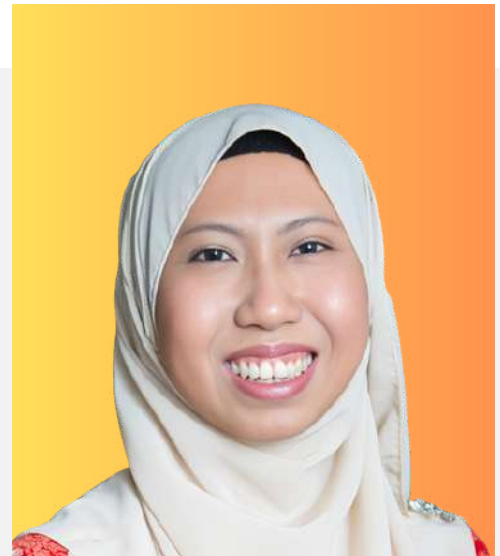
Accident and Consequences Modelling for Hydrogen Storage in Stationary and Mobile

Dr. Norafneeza Norazhar

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The transportation sector heavily relies on fossil-based fuels, contributing significantly to the escalating concentration of pollutants and greenhouse gases in the atmosphere. Hydrogen emerges as a promising and clean energy carrier to address such environmental challenges and the increasing energy demand. Unlike fossil fuels, hydrogen offers a cleaner transportation option due to its unique characteristics, including high energy density, a substantial calorific value, cost-effectiveness, and diverse production methods. With these attributes, hydrogen has the potential to serve as a viable and eco-friendly substitute, capable of entirely replacing fossil fuels in internal combustion engines. However, hydrogen storage and transport are significant challenges because the hydrogen characteristics limit the technology options. This study presents the consequence modelling of hydrogen release and explosion using ALOHA and HyRAM+ software. The hydrogen release and explosion are modelled in stationary and mobile modes. ALOHA illustrated the release rate, burn rate, toxic threat zone, flammable threat zone, thermal radiation threat zone and overpressure threat zone. HyRAM software models a jet flame temperature, trajectory, heat flux, and overpressure. The three most dangerous scenarios were hydrogen leaking without burning for refuelling gas station, BLEVE for hydrogen production storage and liquid hydrogen trailer. The safe area to locate hydrogen storage away from residential areas is 274m for refuelling gas station, 757 m for hydrogen production storage and liquid hydrogen trailer. The hydrogen-powered vehicle has the most minor threat zone as their tank volume is only 62.4 L, and the release of hazardous chemicals into the environment is the least. BLEVE threat zone, where the most significant effect distance was transferred to Google Earth. There may be severe exposures and domino effects on the people around. For hydrogen production, the radius of the overpressure area is more than 140 m, which is affected by the delayed ignition of the leaking gaseous hydrogen over 5 kPa. This area's radius is approximately 40 m of the region affected by overpressure higher than 16 kPa, which has risks of structure collapse, possible fatality by being projected against obstacles, and skin lacerations by missiles. The findings have contributed to the understanding and managing of accidents and consequences in hydrogen storage systems, enhancing the safety and sustainability of this emerging technology.



Biography

Dr. Norafneeza is also a research fellow at the Center of Hydrogen Energy (CHE) of Institute of Future Energy. She completed a postdoctoral program at Mary Kay O'Connor Process Safety Centre, Texas A&M University in 2023 under supervision of Professor Dr. Faisal Khan. The field of study is human factors, safety, and risk assessment for the process industry. She taught courses of process safety, risk assessment, and human factors to both undergraduate and postgraduate students. In 2023, Dr. Norafneeza Norazhar received a research funding from the Ministry of Higher Education for a project entitled 'Correlating the chemical degradation and the ageing phenomenon of polymer electrolyte membrane (PEM) water electrolysis using Bayesian structural equation modeling'. She wrote articles and published them in reputable journals; Safety Science, Process Safety and Environmental Protection (PSEP), and International Journal of Hydrogen Energy (IJHE).

Invited Presentation 7

OP-052

Towards large area Cu_2SnS_3 thin film by Cost effective and solution-based technique for water treatment and hydrogen production

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In the present work, the photocatalytic activity of heat treated of pure and doped Cu_2SnS_3 (CTS), prepared by the spin coating technique, and its utilization as a catalyst for the degradation of Red reactive azo dye were studied. All samples are treated after deposition in tube furnace adjusted 500 °C with flow of argon and presence of sulfur for 60 min. After treatment and cooling, the structural, morphological, and optical properties of the samples were evaluated. The degradation of azo dyes was used to evaluate the photocatalytic activity of the pure and doped CTS thin film under day light irradiation. When compared to pure CTS, the doped CTS demonstrated increased in photocatalytic activity. The improved photocatalysis is due to reduced recombination of generated charge carriers via dopant in CTS. The simple and well-organized spin coating method for catalyst preparation will be more suited to industrial production for water treatment and hydrogen production.



Biography

Prof. Dr. Fawzy Abdel Hamid Mahmoud Hassan, graduated from faculty of science - Ain Shams University in 1991 (Physics), gained his master's degree also from Ain Shams university in solid state physics 1998, and obtained his Ph.D. in solid-state physics from the National University of Kazakhstan in 2005 under the title "modification of electronic properties of diamond like carbon thin film". He joined National research centre, Egypt in 1993 as a research Assistant in the Solar Energy department but in 1995 he moved to solid state physics department and got position of Professor in the Department of solid-state physics from 2021 until now. His research is concerned on thin film technology, nanomaterials, new materials and their applications in the field of solar energy, as well as environmental pollution detectors and treatments. He attended many scientific conferences related to nanotechnology, where he is one of the ISESCO experts in this field, and he was officially invited to speak at many ISESCO conferences in this field. He has scientific relations and research projects with many international laboratories in the materials sciences and its applications in Energy and environmental applications. He is a reviewer of both ASRT-Egypt and science and technology fund -Egypt. Also he is a reviewer of many high impacted international scientific journals in material science and its applications.

Invited Presentation 8

OP-051

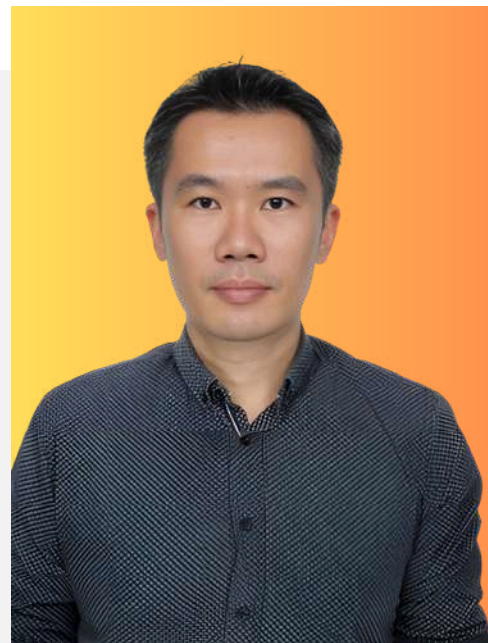
Hybrid Organic-Inorganic Hydrides for Reversible Hydrogen Storage

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Gasification is a thermochemical conversion to produce syngas, which is a mixture of Hydrogen, Carbon Dioxide, Carbon Monoxide, and Methane. Hydrogen is a clean and efficient energy carrier that has a wide range of uses, from powering fuel cells to industrial processes. Malaysia has a strategy to shift into utilizing Hydrogen and since Malaysia generates a huge amount of biomass waste annually, the gasification of biomass waste may offer a sustainable way for Malaysia to commit to its goals. In 2022, Malaysia produced around 182.5 million tonnes of biomass waste, spread across Peninsular Malaysia, Sabah, and Sarawak, which can generate approximately 7.2 million tonnes of Hydrogen. This study aims to investigate the feasibility of performing a biomass gasification process to obtain Hydrogen and downscale it for local and rural implementation. Gasification using pure Oxygen can increase the yield of Hydrogen in the syngas. Moreover, an economic analysis was conducted to compare the deployment of either electrolyzer or air separation unit to obtain the Oxygen to ensure that the whole process is economically viable.



Biography

Chua Yong Shen received his Ph.D. degree in Chemistry at the National University of Singapore in 2011 under the supervision of Prof. Chen Ping. After graduation, he joined Dalian Institute of Chemical Physics (DICP) as a Postdoctoral Research Fellow. During his postdoctoral research, he visited the National Institute of Standards and Technology (NIST) for 10 months as a Guest Researcher. He is currently serving as a senior lecturer at the School of Chemical Sciences, Universiti Sains Malaysia (USM) and was recently appointed as a visiting professor at Guilin University of Electronic Technology, China. His current research interest focuses on various hydrides for hydrogen storage, including metal hydrides, chemical hydrides, hybrid organic-inorganic hydrides and liquid organic hydrogen carriers. He has led several research projects funded internally and externally. He has published more than 40 articles with a total citations of 2700.

Invited Presentation 9

OP-028

Levelized Cost Analysis of Solar Hydrogen Production

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Green hydrogen is gaining traction with people around the world who see the opportunity to generate hydrogen from renewable energy. Producing 70 million tonnes of electrolyzed hydrogen requires 3,600 TWh of electricity, which is more than the combined annual energy production of the European Union. Instead of employing carbon-free energy as a source, hydrogen technology transfers it as a chemical energy carrier that is used to alter, store, and then release energy. It's becoming one of the paths to near-total decarbonisation as low-carbon fuels. The hydrogen market size is about USD 2.5 trillion in 2021, with USD 15 trillion in global investment and multiple expected growths. However, the levelized cost of integration between hydrogen and renewable energy systems is still high. Thus, green hydrogen currently makes up a small percentage of total hydrogen due to its cost and several hurdles such as enormous system size, and supply shortages brought on by renewable energy intermittent issues.



Biography

Dr. Norashikin Ahmad Ludin holds a PhD in Chemistry (Solar Photovoltaic Technology) from the University of Wales, UK, and is currently an Associate Professor and Senior Research Fellow at the Solar Energy Research Institute, UKM. With over 20 years of experience in renewable energy (RE), her expertise includes advanced materials for solar photovoltaics and impact analysis of these technologies. Her research also covers RE policy, life cycle assessment, and end-of-life management of solar PV. Dr. Norashikin has published over 100 high-impact papers, led international and national research projects totaling USD 2.5 million, and supervised more than 40 postgraduate students. She has served as a Visiting Professor at Claremont McKenna College, USA, and a Visiting Researcher at Tokyo University of Science, Japan. Her engagements include roles with ASEAN COSTI, MITI, and ERIA, and she is a Certified Energy Manager under ASEAN Centre of Energy. Recently, she completed an Executive Education in Circular Economy and Sustainability Strategies at Cambridge University, UK.

Invited Presentation 10

OP-026

Physicochemical and Electrocatalytic Properties of NiMoO₄/Ni in AEM Water Electrolysis

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The development of sustainable electrocatalysts is essential for the advancement of anion exchange membrane water electrolysis (AEMWE) technologies. Nickel molybdate-based catalysts may improve the efficiency of hydrogen evolution reaction (HER) during alkaline water electrolysis. This study investigated the influence of thermal reduction temperature on the physicochemical properties of synthesized NiMoO₄-based catalyst via solution combustion synthesis (SCS) and its performance in half-cell HER and single-cell AEMWE. The optimal conditions for stable and active HER electrocatalysts were determined by investigating synthesized NiMoO₄ catalysts at 450 °C, 550 °C and 750 °C. A NiMoO₄ catalyst was characterized at different reduction temperatures through X-ray diffractometer (XRD), field emission scanning electron microscopy (FESEM), energy-dispersive spectroscopy (EDS) and Brunauer–Emmett–Teller (BET) analysis. Results revealed that the NiMoO₄-450/Ni cathode indicated the highest performance of 1 A/cm² current density at 2.2 V and the NiMoO₄-550/Ni cathode became the most stable performance among the catalysts, attaining. The average current density of NiMoO₄-550/Ni fluctuated by only 22% from 24 h to 100 h. The improved stability of the catalyst could lead to increased hydrogen production rates and higher overall system efficiency.



Biography

Dr. Rozan Mohamad Yunus is an Associate Professor and Senior Research Fellow at the Fuel Cell Institute, Universiti Kebangsaan Malaysia. She earned her bachelor's and master's degrees in Material Science from Universiti Kebangsaan Malaysia in 2005 and 2011, respectively. She then completed her Ph.D. in Material Engineering at Kyushu University, Japan, in 2016. Dr. Rozan's current research interest is the development of advanced materials, such as electrocatalysts and photoelectrodes, for water splitting and the green hydrogen production. Her innovative work has garnered significant research funding from both government and industrial sources, strengthening her contributions to this field. As a project leader, she has successfully managed government and industry grants related to hydrogen energy, totalling RM 4.1 million between 2016 and 2024. Beyond her research endeavours, Dr. Rozan is an active member of the Malaysian Association of Hydrogen Energy (MAHE) and the Malaysia Solid State Science and Technology Association (MASS). Her involvement in these organizations underscores her commitment to advancing the field of hydrogen energy and materials science in Malaysia.

Invited Presentation 11

OP-058

Advanced Ternary Photocatalyst: Ce-Doped Bi_2O_3 Integrated with Biochar for Enhanced Tetracycline Degradation

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The escalating environmental concerns posed by the persistence of antibiotics and organic dyes in industrial effluents demand the development of efficient and cost-effective contaminant removal strategies. This study addresses the urgent demand for advanced semiconductor photocatalysts by fabricating a novel biochar-based Bi_2O_3 composite doped with Cerium (Ce) using spent coffee grounds as a biochar source. The ternary composite, $\text{Bi}_2\text{O}_3\text{-BC/Ce}_{3.0}$, was synthesised via a solvothermal method, with varying molar ratios of Ce, and selected as the optimal candidate for in-depth physiochemical characterisation alongside pristine Bi_2O_3 . Results confirmed the well-defined microstructure of the composite. At the same time, UV-Diffuse Reflectance Spectroscopy and photoluminescence analyses demonstrated a significant reduction in the band gap from 3.21 to 2.19 eV in the optimized sample, accompanied by a decreased electron-hole recombination rate. The photocatalytic efficiency was evaluated using Tetracycline (TC) degradation under direct sunlight over 90 minutes. The $\text{Bi}_2\text{O}_3\text{-BC/Ce}_{3.0}$ composite exhibited superior degradation efficiency (95.34%) compared to pure Bi_2O_3 (53.87%) under optimized conditions, with degradation rate constants of 0.00527 min^{-1} and 0.0196 min^{-1} , respectively. Scavenging experiments highlighted the dominant roles of holes (h^+) and superoxide radicals ($\text{O}_2^{\bullet-}$) in the degradation process, with negligible contribution from hydroxyl radicals (OH^{\bullet}). Furthermore, the composite exhibited excellent reusability, maintaining stability and effectiveness over ten cycles, with only a slight decrease in efficiency from 94% to 74%. This work underscores the potential of $\text{Bi}_2\text{O}_3\text{-BC/Ce}_{3.0}$ as a highly effective and durable photocatalyst for large-scale environmental applications.



Biography

Dr. Noor Haida Mohd Kaus is an Associate Professor at the School of Chemical Sciences, Universiti Sains Malaysia. She earned her BSc in Applied Chemistry (2005) and MSc in Advanced Materials (2008) from Universiti Teknologi MARA, Malaysia, and her PhD in Chemistry (2012) from the University of Bristol, UK. Internationally recognized in Nanomaterials and Photocatalysis, her research focuses on sustainable nanomaterials for environmental remediation and energy generation. She has supervised 7 PhD and 12 Master's students, published over 80 ISI journal articles with an H-index of 24 (WoS) & 25 (Google Scholar), and received more than 6000 citations. Dr. Haida has led 10 research projects, including 3 international grants, and co-investigated 25 others, totaling RM3.5 million (USD 700,000). Her team developed a composite photocatalyst for water treatment and a cost-effective catalyst for biodiesel production. She serves on evaluation panels for national and international grants and has been a keynote speaker at numerous conferences. Her work has earned several innovation awards and international recognitions, including a Cross-Appointment as an Associate Professor at Nagaoka University of Technology, Japan (2016-2026). Dr. Haida is actively seeking collaborators and students in photocatalysis, wastewater treatment, bioactive nanocolloids, and photofunctional materials..

Invited Presentation 12

OP-022

Heterogeneous Catalysis for CO₂ Conversion into Chemicals and Fuels

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Catalytic conversion of CO₂ into chemicals and fuels is a viable method to reduce carbon emissions and achieve carbon neutrality. Through thermal catalysis, electrocatalysis, and photo(electro)catalysis, CO₂ can be converted into a wide range of valuable products, including CO, formic acid, methanol, methane, ethanol, acetic acid, propanol, light olefins, aromatics, and gasoline, as well as fine chemicals. In this study, we summarize the recent progress in heterogeneous catalysis for CO₂ conversion into chemicals and fuels and highlight some representative studies of different conversion routes. The structure–performance correlations of typical catalytic materials used for the CO₂ conversion reactions have been revealed by combining advanced in situ spectroscopy and microscopy characterizations and. Catalytic selectivity toward a single CO₂ reduction product/fraction should be further improved at an industrially relevant CO₂ conversion rate with considerable stability in the future.



Biography

Sharifah Najiha is a research fellow at the Fuel Cell Institute, Universiti Kebangsaan Malaysia. She earned her Bachelor's degree in Industrial Chemistry in 2009 and her Ph.D. in Chemistry in 2014, both from Universiti Teknologi Malaysia. Her current research focuses on developing and modifying novel catalysts for CO₂ conversion and utilization, hydrogen production and storage, as well as fuel cell applications.

Invited Presentation 13

OP-029

Enhanced Bimetallic Alloy Catalysts: A DFT Study on Structural, Electronic, and Adsorption Properties

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Bimetallic alloys have shown superior performance over monometallic noble metal catalysts in conversion from alcohol to valuable product and oxygen reduction reaction. However, catalyst performance remains a challenge and requires modification. This study investigates five catalyst models—Pd (111), Ag (111), Pd₃Ag (111), PdAg (111), and PdAg₃ (111)—focusing on their structural, electronic, and adsorption properties through density functional theory (DFT) analysis. The structural and electronic properties of the modified catalyst model show the ligand and strain effect on the alloy with the addition of silver as second metal promotes the adsorption capability; however, the catalytic activity heavily depends on the alloy composition. The addition of silver (Ag) in these alloys enhances adsorption capabilities, but the catalytic activity varies with alloy composition. Pd₃Ag (111) exhibited the best adsorption properties for atoms and alcohol/polyol molecules, including methanol, ethanol, and glycerol. It also showed strong catalytic activity for the oxygen reduction reaction (ORR), making it a suitable candidate for direct liquid fuel cells. Ag's inclusion significantly improved glycerol adsorption, promoting its oxidation reaction, especially in direct glycerol fuel cells (DGFCs). DFT calculations revealed that the addition of Ag to Pd catalysts facilitates the glycerol oxidation reaction (GEOR), with primary carbon oxidation leading to intermediary products like glyceraldehyde and glyceric acid. Ag also aids in C-C bond cleavage, increasing selectivity for high-value products such as glycolic and oxalic acids. This study's findings provide insights into designing better alloy catalysts for alcohol and polyol fuels in DLFC applications, offering potential pathways for future improvements.



Biography

Nabila A Karim is a seasoned research fellow at the Fuel Cell Institute of the National University of Malaysia, where she has been a pivotal figure since 2017. With a Ph.D. in Fuel Cell Engineering, Nabila's research is deeply rooted in Density Functional Theory (DFT) and computational modeling, areas in which she has made substantial contributions. Her expertise lies in using DFT to investigate the electronic properties and catalytic behaviors of advanced materials, which are crucial for enhancing the performance of fuel cells and other energy conversion technologies. Nabila's work focuses on the theoretical analysis and modeling of catalytic systems, providing insights into the fundamental mechanisms that drive reactions at the molecular level. This approach has allowed her to design and optimize new catalysts with improved efficiency and durability, particularly in applications related to hydrogen production and fuel cell technologies. Her research not only advances the understanding of catalytic processes but also guides the experimental development of materials, bridging the gap between theory and practical application.

OP-002

Maximizing Hydrogen Recovery: Integrating Dark Fermentation with Solar-Powered Microbial Electrolysis Cell System

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Abstract

Hydrogen, acclaimed for its eco-friendliness and potential as a sustainable energy carrier, has attracted considerable scholarly attention. Its production from diverse domestic resources, including solar and wind power, offers a promising avenue for renewable energy. Dark fermentation, recognized as a green technology leveraging waste streams, provides a pathway for hydrogen production. However, its efficiency is constrained by metabolic limitations and microbial dynamics. Microbial electrolysis cells (MECs) present an opportunity to further exploit energy from fermentative effluents, resembling water electrolysis albeit with reduced energy input. The integration of fermentative-MEC systems holds significant promise for optimizing energy recovery and hydrogen output. Despite the support from bioanode oxidation reactions, MECs still necessitate external power for hydrogen evolution on the cathode. This study endeavors to bridge this energy gap by harnessing solar energy during daylight hours to power MEC operations. Commencing with system design amalgamating dark fermentation, solar panels, and MECs, the study progresses to test and operate the integrated system in batch and fed-batch modes. Streamlined control units optimize effluent discharge and hydrogen yield, establishing a closed-loop, self-sustaining system for hydrogen generation from wastewater. The utilization of palm oil mill effluent, abundant in Malaysia and rich in organics, serves as an ideal model for system operation.

Keywords: hydrogen production, palm oil mill effluent, dark fermentation, microbial electrolysis cell, solar energy.

OP-004

Hybrid Perovskite Solar Cells: Properties, Fabrication Techniques, and Commercialization Challenges

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Abstract

Hybrid perovskite solar cells (HPSCs) have gained significant attention as a promising technology for efficient and cost-effective renewable energy generation. With the increasing demand for sustainable and natural resources, HPSCs offer a viable solution for addressing the world's energy challenges. This review article provides a comprehensive understanding of the properties and working nature of HPSCs, their low-cost fabrication techniques, and the challenges faced by them during commercialization. The review aims to highlight the potential of HPSCs in revolutionizing the renewable energy landscape, providing insights into their properties and challenges. The analysis is based on a thorough examination of the literature on HPSCs and their comparison to traditional silicon-based solar panels. The findings are relevant for advancing the field of photovoltaics and offer essential considerations for policymakers, practitioners, and researchers seeking sustainable and environmentally friendly energy solutions. Overall, this review emphasizes the potential of HPSCs as a promising technology for efficient and cost-effective renewable energy generation, paving the way for a cleaner and greener future.

Keywords: hybrid perovskite solar cells; renewable energy; fabrication; commercialization

OP-005

Bi₂O₃ Particles Decorated on Porous g-C₃N₄ Sheets: Enhanced Photocatalytic Activity through a Direct Z-scheme Mechanism for Degradation of Reactive Black 5 under UV-vis Light

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Abstract

Synthesis of a composite photocatalyst is a good approach to utilize higher portion of solar spectrum and improves separation of electron-hole pairs. Herein, a novel Bi₂O₃/porous g-C₃N₄ synthesized using impregnation method showed dramatic photo-activity improvement under irradiation of UV-vis light. Further characterization by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), high-resolution transmission electron microscopy (HRTEM), Fourier transform infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) proved the existence of both g-C₃N₄ and Bi₂O₃ in which Bi₂O₃ particles are decorated on porous g-C₃N₄ sheets. Photocatalytic activity test of Bi₂O₃/porous g-C₃N₄ composites shows that 9 wt% Bi₂O₃/porous g-C₃N₄ is the best photocatalyst with 84 % of Reactive Black 5 (RB 5) degradation under 120 min of UV-vis light. It was confirmed that the photocatalytic activity improvement is due to the reduction of electron-hole recombination and wider absorption of light which were proven using photoluminescence (PL) and UV-vis diffuse reflectance spectroscopy (DRS), while surface area plays an insignificant role in the photocatalytic performance. In addition, process parameters studies concluded that 9 wt% Bi₂O₃/porous g-C₃N₄ worked best in RB 5 with concentration of 10 ppm, pH 5.7 and by using 1 g/L photocatalyst loading. From radicals quenching test, superoxide radical (O₂^{•-}) was found to be the most active radical which mineralizes RB 5 by following the mechanism of direct Z- scheme pathway. Lastly, 9 wt% Bi₂O₃/porous g-C₃N₄ is stable and preserved its photocatalytic activity up to three times for degradation of RB 5.

Keywords: g-C₃N₄; Bi₂O₃; Photocatalysis; Reactive Black 5

OP-006

ZnO with Engineered Surface Defects as a Competent Photocatalyst for CO₂ Photoreduction into Valuable Fuels under Simulated Solar Light Irradiation

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Abstract

Photocatalysis is one of the eco-friendly methods in greenhouse gases abatement by utilizing renewable resources such as sunlight. This study examined defective ZnO nanoparticles that serve as carbon dioxide (CO₂) adsorption and activation sites in photocatalytic reactions. The defective ZnO nanoparticles were synthesized via a facile precipitation-hydrothermal method by only controlling the concentration of NaOH as the precipitating agent. The rough surface of ZnO were formed due to the heating treatment, where it conveniently removed the attached inorganic molecules on ZnO surfaces. The roughness surface of ZnO was observed by using Transmission Electron Microscopy (TEM) analysis, in which the pores with bright spot can be observed. Additionally, the defects originating from oxygen vacancies (VO), zinc interstitials (Zni) and carbonates groups (CO₃²⁻) were successfully optimized over variation of NaOH concentrations proven by Photoluminescence (PL) and X-ray photoelectron Spectroscopy (XPS) analysis. Here, 1: 4 ZnO exhibited the highest CH₄ yield (1.3 × 10⁻¹ μmol) and 3-fold production than commercial ZnO (4.8 × 10⁻² μmol). The reusability of 1: 4 ZnO was demonstrated by conducting 4 cycles of stability test, which revealed a robust photocatalyst of 7.7% performance reduction after 4th cycle. A schematic mechanism pertaining to the novel defective ZnO nanoparticles in CO₂ photoreduction to valuable fuels was proposed in this study, which undoubtedly will contribute a positive effect to industry's long-term sustainability.

Keywords: CO₂ reduction; Photocatalyst; ZnO; CH₄

OP-007

Oxygen Reduction Reaction on Single-Atom Catalyst from Density Functional Theory Combined with an Implicit Solvation Model

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Abstract

It has been well established that the single-atom catalyst, particularly the transition metal (TM = Fe and Co) embedded in N-doped graphene, has the potential to reduce O₂ to H₂O with appreciable activity and stability. However, substantial improvement in the oxygen reduction reaction (ORR) activity at lower overpotential are still required. The atomistic simulation that takes into account the electrochemical environment, i.e., electrode potential and electrical double-layer (EDL), are desirable to better understand the underlying reaction mechanism of the ORR. Here, we present a density functional theory study on the mechanism of ORR on the Fe-N₄-C and Co-N₄-C in contact with an acidic solution under an applied potential, enabled by the effective screening medium method combined with the reference interaction site model (ESM-RISM). We found the solvent effect is essential in modelling the ORR, as the potential-determining step (PDS) changes from *O → *OH (O₂ → *OOH) to *OH → H₂O (I) (*OH → H₂O (I)) for Fe-N₄-C (Co-N₄-C) when the implicit solvent is introduced. We also found, with the constant potential method combined with the ESM-RISM, the reaction intermediates become competitive, and the resulting PDSs are changes from *O → *OH and O₂ (g) → *OOH for Fe-N₄-C and Co-N₄-C, respectively. The calculated limiting potentials are comparable for both Fe-N₄-C and Co-N₄-C, in contrast to the results obtained using the constant (neutral) charge simulation in which the superior catalytic activity of Co-N₄-C has been predicted. The origin of the discrepancy between these results is mainly the charge state (different from the neutral one) at a fixed electrode potential, which can be determined through the constant potential method with ESM-RISM. This work clarifies the roles of electrolyte solutions within the RISM framework and demonstrates the importance of the variable charge state through the constant potential calculation.

Keywords: single-atom catalyst; oxygen reduction reaction; constant-potential simulation; ESM-RISM; fuel cell application

OP-008

Temperature-Tuned Hydrothermal Synthesis on Porous Substrate: Boosting PEC Efficiency of ZnO/Graphene/Nickel foam

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Abstract

Zinc oxide (ZnO) as a photoanode material has intrinsic limitations, such as a wide band gap and high recombination rate of electron–hole pairs. This limit the photoelectrochemical (PEC) performance. In this study, ZnO is grow on graphene/nickel foam (Gr/Ni-foam) by varying reaction temperatures during the hydrothermal method. Results indicate that ZnO/Gr/Ni-foam exhibits an outstanding PEC performance at higher temperatures (200 °C). In addition, the presence of Gr/Ni-foam enhances the light absorption capability and band gap energy (E_g) of ZnO. Hence, ZnO/Gr/Ni-foam greatly increases the photocurrent density (24.07 mA cm⁻²) compared to Ni-foam at 1.23 V vs RHE in 0.5 M Na₂SO₃. This study describes an innovative strategy for developing sustainable photoanodes for PEC water splitting.

Keywords: *Zinc oxide, Graphene, Nickel foam, Porous substrate, Photoelectrochemical performance*

OP-009

Synthesis and Characterization of Ni-doped Natural Zeolite Catalyst by Wet Impregnation Method

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Abstract

The development of efficient and sustainable catalysts is crucial for advancing catalytic processes in various industrial applications. This study presents the synthesis and characterization of nickel (Ni)-doped natural zeolite catalysts using the wet impregnation method. Natural zeolite, a readily available and cost-effective aluminosilicate mineral, was chosen as the support material for Ni impregnation. The synthesis process involved impregnating natural zeolite with an aqueous solution of NiSO₄ MHP (Mixed Hydroxide Precipitate) at a zeolite-to-nickel ratio of 50 w/w, followed by drying and calcination at 500°C. Comprehensive characterization of the Ni-doped zeolite catalysts was performed using X-ray Fluorescence (XRF), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and Brunauer-Emmett-Teller (BET) surface area analysis. XRF analysis confirmed successful nickel impregnation into the zeolite pores at a concentration of 0.30%. XRD analysis verified the preservation of the zeolite structure post-impregnation and the successful incorporation of Ni species. FTIR spectra indicated no significant alteration in the zeolite's framework post-doping, suggesting that structural integrity was maintained. BET surface area measurements showed a decrease from 91.72 to 60.79 m²/g upon Ni doping, attributed to pore blockage by Ni particles. This study highlights the potential of Ni-doped natural zeolite catalysts in various industrial applications, offering a cost-effective and sustainable alternative to conventional catalysts. Further research into optimizing Ni loading and exploring the catalytic mechanisms is warranted to fully harness the capabilities of these novel materials.

Keywords: *Catalyst; Nickel-doped Zeolite; Synthesis; Wet Impregnation*

OP-012

Synthesis and Fabrication of TiO₂/rGO Nanotube-Based Photoanodes for Photoelectrochemical cells

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Abstract

The use of titanium dioxide, TiO₂ as a photoanode material for hydrogen production via water splitting has garnered significant attention in recent decades. TiO₂ is a promising choice due to its low toxicity, excellent chemical stability, and suitable band gap position for water reduction. However, the wide band gap energy of TiO₂ (3.2 eV) limits its ability to effectively absorb visible light, and the high recombination rate of photoexcited charge carriers results in low quantum efficiency. To address these limitations, various material modifications were explored in order to enhance the photocatalytic performance of TiO₂. In this work, the TiO₂ nanotubes was synthesis by anodization of a Ti mesh and subsequently deposited reduced graphene oxide (rGO) on the nanotubes using an electrodeposition method to create a 3D structured composite. The crystal structure of the anatase TiO₂ nanotubes and the presence of rGO were confirmed through characterization techniques such as FE-SEM, EDX, XRD, HR-TEM, and Raman spectroscopy. The photoelectrochemical performance of the TiO₂/rGO composite was evaluated by measuring the photocurrent density in a 1M KOH electrolyte. It was found that the TiO₂ nanotubes with 0.5 g/L rGO deposition exhibited the optimum photoelectrochemical result, with a 5-fold increase in photocatalytic activity compared to the bare TiO₂ nanotubes under solar light irradiation at 0.6 V.

Keywords: photocatalytic, carbon nitride, graphene oxide, nickel sulphide,

OP-013

Sustainable Direct Recycling of Spent Lithium-ion Batteries Using Green Organic Acid and Flame-Assisted Spray Pyrolysis

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Abstract

The exponential market growth in lithium-ion batteries (LIBs) will cause several problems, such as supplying the high demand for raw materials in manufacturing and having an environmental impact on end-of-life LIBs. Recently, the direct recycling of spent lithium-ion batteries has become more popular to tackle these problems due to the closed-lope circular model that uses less chemical agents and energy to make the new active materials. In this work, the recovery of new cathode active material uses organic acid (acetic acid) as a leachate agent through direct synthesis on fame-assisted spray pyrolysis (FASP). The various hydrometallurgical processes, such as variation of acid concentration, solid-to-liquid ratio and temperature, were analyzed. The optimum process was selected for the 1.25 M of acetic acid with a solid-to-liquid ratio of 30 gr/L and temperature 70°C. The leaching efficiencies for Li(I), Ni(II), Mn(II), and Co (II) were 87,16%; 64,34%; 82,89%; and 99,24%, respectively. The X-ray diffraction (XRD) analysis shows that the synthesized cathode with the FASP method has a good crystallization rate without any impurities detected. The morphology and particle size investigated by Scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX) and Particle size analysis (PSA) method revealed that the synthesis of nanoparticles by FASP method showed a spherical shape morphology with typical polycrystalline aggregates and had a particle size distribution in the range of 200- 400 nm.

Keywords: *Spent lithium-ion batteries; Hydrometallurgy; Organic acid; Flame Assisted Spray Pyrolysis*

OP-015

Study of the Potential Use of Plastic Waste as a Bipolar Plate Material in PEMFC Applications Through Fluid-Structure Interaction Analysis

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Abstract

Bipolar plates are essential in Proton Exchange Membrane Fuel Cells (PEMFCs) for maintaining structural integrity and facilitating electrochemical reactions. Traditionally, these plates are made from expensive and resource-intensive materials such as graphite or metal composites. This research explores the potential of using compressed waste plastic as an alternative material for bipolar plates. The study focuses on the mechanical viability of compressed waste plastic, which offers a cost-effective, ease of manufactured and environmentally friendly alternative. The main sources of waste plastic are from household and industrial production waste. Waste plastics are processed through extrusion and compression molding to make specimens for experimental testing, which have successfully demonstrated several values such as tensile strength, compression resistance, density, and fatigue cycle performance. Fluid-Structure Interaction (FSI) analysis employed to simulate the interaction between fluid flow and the structural behavior of bipolar plates made from waste plastic under typical PEMFC operating conditions. This method provides a comprehensive assessment of both mechanical stability and fluid dynamics within the fuel cell. The findings demonstrate that compressed waste plastic exhibits promising mechanical properties, including adequate strength and flexibility, making it capable of withstanding the operational stresses in PEMFCs and visualize the required flow fluid dynamics for fuel cell operation. This study presents a novel approach to repurposing waste plastic, addressing both environmental waste issues and reducing material costs in PEMFC applications.

Keywords: *Bipolar plates; waste plastic properties; fluid-structure interaction*

OP-017

Catalytic pyrolysis reaction on Ni-CeO₂ (111) for hydrogen-rich gas: DFT study

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Abstract

The production of hydrogen (H₂) from biomass pyrolysis presents significant advantages, including the utilization of renewable energy sources, zero-carbon emissions, cost-effectiveness, and high efficiency. Incorporating Ni-based catalysts into the biomass pyrolysis process can enhance the reaction rate and reduce coke formation. However, catalyst deactivation due to carbon deposition, poisoning, and sintering remains a critical challenge. Investigating the impact of catalysts on the reaction mechanism is essential for optimizing the biomass pyrolysis process. This study focuses on the Ni-CeO₂ (111) catalyst model to further explore these effects. The activation energy (E_a) for the rate-determining steps of the water-carbon reaction, Boudouard reaction, methane steam reforming reaction, and water-gas shift reaction were examined. Density Functional Theory (DFT) results revealed that the order of E_a for key reactions in H₂ production on the Ni-CeO₂ (111) catalyst is as follows: water-carbon reaction < Boudouard reaction < methane steam reforming reaction < water-gas shift reaction. These findings indicate that the water-gas shift reaction is the crucial control step in the process. The results of this study contribute to the understanding the catalytic mechanisms involved in biomass pyrolysis, particularly in the context of H₂ production. By identifying the rate-determining steps and their corresponding activation energies, this research provides valuable insights for the design and development of more efficient catalysts. Ultimately, these findings can lead to optimized biomass pyrolysis processes, contributing to the advancement of sustainable and renewable energy technologies.

Keywords: DFT; biomass; pyrolysis; hydrogen; nickel

OP-019

Advancing PEC Water Splitting Performance with Nickel-Based Protective Coating (NiO) and Co-Catalyst Layer (NiFe-LDH) on Cu₂O/CuO Photoelectrodes.

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Abstract

Cuprous oxide (Cu₂O) is a popular choice as a photocathode for green hydrogen production via photoelectrochemical (PEC) water splitting because of its appropriate bandgap. However, it is plagued by inadequate stability, which impedes its overall effectiveness. This study examines how a nickel-based protective and co-catalyst layer improves the performance of Cu₂O photocathode for water splitting application. NiO is an ideal protective material for Cu₂O thanks to its large bandgap of 3.5 eV, meanwhile, NiFe-LDH has been shown to be very promising hydrogen evolution reaction (HER) electrocatalyst for water splitting. In this work, we address these issues by a strategy to simultaneously protect Cu₂O and enhance its PEC water reduction performance, wherein the CuO layer that comes from the deposited Cu₂O after annealing will enhance the charge separation process, and the NiO layer will increase the stability of the photoelectrode. The Cu₂O/CuO/NiO/NiFe-LDH photoelectrodes prepared via electrodeposition and thermal oxidation methods are thoroughly analysed for their structural, optical, and electrochemical properties. The performance of the Cu₂O/CuO/NiO/NiFe-LDH photoelectrode were expected to be significantly improved compared to the bare Cu₂O/CuO photoelectrodes. The Cu₂O/CuO/NiO/NiFe-LDH photoelectrodes also demonstrate better charge transfer and decreased charge recombination. This research offers vital insights on how nickel-based protective and co-catalyst coatings might enhance the performance of Cu₂O photoelectrodes for water splitting applications, thus advancing renewable energy technology.

Keywords: copper oxide; protective layer; co-catalyst layer; nickel-based; photoelectrochemical water splitting

OP-023

Enhanced Hydrogen Production using Co, Cu, and Ni-doped TiO₂ photoanodes in Photoelectrochemical Cells

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Abstract

This study explores the efficacy of photoelectrochemical (PEC) cells employing Co, Cu, and Ni-doped TiO₂ as photocatalysts for hydrogen production. Pure TiO₂ was synthesized via the sol-gel method and subsequently doped with 5% by weight of Co, Cu, and Ni ions through the deposition-precipitation method. The resulting nanomaterials were characterized using Field Emission Scanning Electron Microscopy (FESEM), Transmission Electron Microscopy (TEM), Diffuse Reflectance UV-Visible Spectroscopy (DR-UV-Vis), and X-ray Photoelectron Spectroscopy (XPS). FESEM and TEM images revealed semi-spherical particles with slight agglomerations and an average size range of 63 to 65 nm. UV-Vis DRS indicated a reduction in the bandgap below 3.2 eV, leading to a redshift and enhanced optical absorption in the UV-visible region. XRD patterns confirmed the anatase phase of TiO₂ and its doped variants, consistent with JCPDS 21-1272. XPS data confirmed the successful deposition of metallic ions and the presence of various valence states in the photocatalysts. Photocatalytic performance was evaluated in a 2M KOH solution with 5% glycerol under illumination from a 500W halogen lamp. The setup included a 1 cm² photoanode area, a platinum cathode, and an Ag/AgCl reference electrode. Among the tested materials, Ni/TiO₂ exhibited the highest hydrogen production (19 mL), followed by Co/TiO₂ and Cu/TiO₂. Electrochemical Impedance Spectroscopy (EIS) showed Ni/TiO₂ had the lowest charge transfer resistance, while Linear Sweep Voltammetry (LSV) and Cyclic Voltammetry (CV) measurements indicated the highest photocurrent density and conductivity, respectively. In conclusion, Ni/TiO₂ outperformed the other doped variants in hydrogen production, demonstrating superior photocatalytic activity, lower charge transfer resistance, and higher conductivity. This makes it a promising candidate for PEC applications in hydrogen generation.

Keywords: Photoelectrochemical cell; hydrogen production; photocatalysts

OP-024

Review on Membrane Electrode Assembly (MEA) Fabrication for Anion Exchange Membrane Water Electrolysis (AEMWE): From Catalyst Ink Preparation to Membrane Electrode Assembly

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Abstract

Sustainable and clean energy are important toward achieving net zero carbon goals and reducing the emission of greenhouse gases and ozone depletion rate. Hence H₂ is known as clean and sustainable. H₂ can be produced in many different methods, but the most promising environmentally friendly method is water splitting. This paper will focus on H₂ production via water electrolysis using an anion exchange membrane water electrolyser (AEMWE). This technology is still in the research and development phase thus it has faced several challenges. However, despite their potential, AEMWE remains in the early stages of development and encounters several obstacles, mainly related to the fabrication of membrane electrode assemblies (MEAs) due to catalyst delamination during operation. There are several steps for MEA fabrication which are materials selection (catalyst, membrane, ionomer, and gas diffusion layer (GDL)), catalyst ink preparation, catalyst coated method, and stacking procedure. Challenges in MEA include catalyst ink preparation to enhance better dispersion and reduce agglomeration by changing solvent and tuning sonication parameters, techniques applied in catalyst coated to minimize the catalyst loss, and catalyst delamination and stacking with the hot press with optimum parameters to avoid membrane microcracking and forming pin hole. MEA fabrication is further discussed in this paper.

Keywords: catalyst ink, MEA, catalyst coating method, AEM water electrolysis

OP-025

Recent progress and new perspective of Borophene-based catalyst for energy application: A Review

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Abstract

Mostly known for its polymorphisms, borophene (2D boron sheets) has emerged as a novel two-dimensional material after the renowned graphene. In contrast to its bulk state, boron, borophene has much more intriguing properties which lead to its comprehensive studies in recent years. However, its experimental realization on borophene synthesis has yet to reach a mature stage, so limited reports are available on its application given its great potential. Moreover, it has gained great attention due to its excellent properties such as tunable electronic structure, high electrical conductivity, and large surface area thus enhancing the catalytic performance through the increased of active sites and charge transfers kinetics making it as an ideal material for use as catalyst in the energy application. Motivated by its first successful experimental realization on metal substrate in 2015 more attempts have been done to produce either pristine borophene or substrate supported borophene for various potential applications. Herein, in this review we discussed the physical properties (electronic and mechanical) and chemical properties of borophene followed by the latest advances in the experimental synthesis strategies and its applications as catalyst in the field of energy. Finally, the main prospects and challenges for the future works are discussed with reference to the practical applications and latest experimental realizations of borophene.

Keywords: borophene, physical properties, catalyst, energy field

OP-027

Impact of oxide growth of TiO₂ on Different Annealing Temperature in Hydrogen Generation on Photoelectrochemical Cells

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Abstract

Photocatalytic water splitting using Titanium Dioxide (TiO₂) as a photocatalyst holds great promise for hydrogen production through solar energy as this method is known for its cleanliness, affordability, and environmental friendliness which aligning with global efforts to transition towards renewable energy sources. However, TiO₂ has high energy band gap with high recombination rate which requires a significant amount of energy to excite an electron from valence band to conduction band. The band gap can be reduced with TiO₂ by annealing under nitrogen-rich condition at varying temperatures of 450°C, 550°C, and 600°C. In this work, the TiO₂ was coated onto ITO glass using spin coating at 2500 rpm and coated substrate was dried at 120°C for 5 minutes. It then undergoes annealing at different temperatures of 450°C, 550°C, and 600°C for 1 hour and slowly cool down at room temperature. Scanning Electron Microscopy was utilized to observe the morphology and measure the thickness of TiO₂ deposited and X-ray Diffraction (XRD) to determine the phase distribution of TiO₂. The PEC has been conducted using 3 electrode system under UVC-LED lamp irradiation. Annealing at different temperatures impacts the surface morphology and causes variations in the phase composition of oxide semiconductor which influence the hydrogen production through water splitting.

Keywords: Annealing; Band gap; Hydrogen; Titanium dioxide, TiO₂

OP-031

Corrosion On Stainless Steel 316l Using Green Inhibitor Garlic Extract (*Allium Sativum*) With NaCl Media

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Abstract

The corrosion process cannot be avoided, but can be minimized by protecting the metal or controlling the rate of corrosion. One way to protect metal from the corrosion process is to use inhibitors. The impact of toxicity and polluting the environment means that the use of conventional inhibitors has become a new problem affecting human health and the ecosystem. Thus, green inhibitors become an alternative to use to produce safe anti-corrosion performance. In this research, a comparative analysis of corrosion rates will be carried out using the potentiodynamic polarization electrochemical method between 316L stainless steel metal and varying concentrations of green inhibitor garlic extract, 0 ml (no inhibitor), 8 ml, 10 ml, and 12 ml in 3.5% NaCl media. to determine the potential of garlic extract as a green inhibitor. The highest inhibition efficiency value was obtained at 82% at a solution concentration volume of 12 ml. So this analysis shows that the greater the concentration of the garlic extract solution, the greater the inhibition efficiency value of the garlic extract. This proves that garlic extract has the potential to inhibit the rate of corrosion in the corrosive NaCl medium

Keywords: Corrosion, Green Inhibitor, SS316, Garlic Extract (*Allium Sativum*),

OP-032

Enhanced Performance of Magnesium-Air Fuel Cells with MnO₂/3D Graphene Composite

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Abstract

Electrochemical energy storage devices such as magnesium-air fuel cell (MAFC) could be improved due to graphene. Graphene has already been widely used as an active and inactive material in rechargeable batteries due to its high specific area, high electrical conductivity, and superior mechanical flexibility. However, graphene's chemical inertness significantly reduces interfacial electron transfer and has a significant impact on ionic and electric conductivity. This study was conducted to synthesize using template and hydrothermal methods and analyze 3D-Graphene (3D-G) and MnO₂/3D-G using X-Ray Diffraction (XRD) and Scanning Electron Microscope (SEM) and will be tested on a single cell MAFC to see the performance of the catalyst that has been produced. The results show the presence of 3D-G and also MnO₂/3D-G and it is found that the 3D-G structure is porous and the MnO₂ nanorods stick to 3D-G uniformly and firmly on the 3D-G surface. In addition, MnO₂/3D-G screened on MAFC air cathode showed a promising performance where the increase was 9.86%. The peak power density value shown at 23.4 mW/cm² compared to commercial MnO which is 21.3 mW/cm². In addition, the MAFC performance test also shows that the current density limit value for MnO₂/3D-G is 23.4 mW/cm², 2.5 V, and 72.1 mA/cm² while for commercial MnO it is 21.3 mW/cm², 1.5 V, and 55.4 mA/cm².

Keywords: *Nanocatalyst; MnO₂/3D; magnesium air fuel cell.*



OP-033

Metal hydride-based catalyst for dehydrogenation of Methylcyclohexane (MCH)

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Abstract

This study investigates the catalytic performance of LaNi₅ alloy, synthesized via six cycles of arc melting at 380 A, in facilitating the reversible dehydrogenation of methylcyclohexane (MCH) as a liquid organic hydrogen carrier (LOHC). The resulting LaNi₅ alloy exhibited high purity and homogeneity, crucial for effective catalysis. Dehydrogenation experiments, conducted at 573 K with 30 mg of LaNi₅ catalyst, achieved a hydrogen storage capacity exceeding 5 wt% over 5 cycles, with near complete MCH conversion to toluene within 8 hours. This exceptional performance, corresponding to a hydrogen release rate of approximately 0.6 wt%/hour, is attributed to the synergistic effect between surface-active nickel species and the LaNi₅ core's intrinsic hydrogen storage capabilities. The findings underscore the potential of LaNi₅-based catalysts in advancing high-efficiency LOHC systems and provide valuable insights into the fundamental mechanisms of hydride-catalyzed hydrogen storage reactions.

Keywords: *hydride-catalysed 1; hydrogen release rate 2; hydrogen storage 3; arc melting 4; toluene 5*

OP-034

Boosted Performance of CO₂-to-Methanol by Controlled Synthesis of Cu@Al₂O₃ Core-Shell Nanostructured Catalyst

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Abstract

By utilizing the core-shell nanostructured catalyst as controlled morphology, constructing thermocatalysts with inversed structures and confined active metals offer advantages for boosting the catalytic performance of CO₂ hydrogenation into methanol fuel. In this study, a porous surface of heterogenous catalyst, Cu@Al₂O₃ was prepared by growing the smaller nanoparticles of alumina shells onto the Cu₂O (Cu⁺/Cu⁰) surfaces. The catalyst shows superior methanol synthesis performance in a slurry batch reactor containing a DMF solvent, requiring only three hours to convert 67% CO₂ feed into 99% methanol and 1% CO, indicating significant thermocatalytic performance of Cu-based catalyst and reaction kinetics characteristic. Furthermore, long-term CO₂ hydrogenation testing also demonstrates the catalyst's outstanding stability. Emphasizing the interfacial interaction between confined active Cu surfaces and porous Al₂O₃ deposition, the study highlights how core-shell morphology collaboratively control the local electronic structure of the Cu@Al₂O₃ and formation of the most stable phase of Cu⁺/Cu⁰, resulting in an efficient Cu-based heterogenous catalyst for thermochemical conversion of CO₂.

Keywords: Copper-based; Methanol; Hydrogenation; New Energy, Core-shell catalyst

OP-035

Revealing the impact of different precursors and solvents for supramolecular complex formation and in-situ C-doping in g-C₃N₄ with enhanced photocatalytic H₂O₂ production

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Abstract

The reinforced light-harvesting capability suppresses photocarrier recombination and increases the specific surface area, representing the possibility of excellent photocatalytic performance for graphitic carbon nitride (CN) photocatalysts. Herein, the remarkable photocatalytic properties of porous carbon-doped g-C₃N₄ (CCN) were enhanced through the incorporation of a supramolecular complex, M-CA-U (melamine-cyanuric acid-urea), in DMSO as the carbon dopant source. Through the diverse characterization methods, the successful formation of the supramolecular g-C₃N₄ using varying polarity of solvent was verified, achieved through a simple hydrothermal/solvothermal process. The CCN-MCAU-DMSO photocatalyst achieved the maximum photocatalytic H₂O₂ production rate, 1.3-fold higher than other prepared samples. The outstanding performances of CCN-MCAU-DMSO were probably attributed to the extended specific surface area, robust visible light response, adjusted electronic band structure, accelerated charge separation, and limited charge recombination. The photocurrent response and photoluminescence spectroscopy analysis confirmed excellent charge carriers and separation. Overall, this work provided a new idea to design and construct high-efficiency porous supramolecular assembly of CCN photocatalysts for photocatalytic studies.

Keywords: C-doped g-C₃N₄; Supramolecular assembly; Photocatalysis; Solvents; H₂O₂ production.

OP-036

Performance Evaluation of P-Block Metal in ORR

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Abstract

The development of efficient and durable oxygen reduction reaction (ORR) catalysts is critical for the advancement of platinum-group-metal (PGM) free fuel cells. The P-block metal (PM) are group by p valence electron with distribution of outer shell is ns_2np_x ($x = 1, 2, 3, 4, 5$). P-block metals can form PM-N-C SACs with good stability due to their atomic radii, which are similar to those of transition metals and Fenton-inactivate as promising catalyst candidates for single-atom active sites for ORR applications especially for fuel cell. This review summarizes recent progress in atomically dispersed p-block-based catalysts, particularly focusing on their application in ORR. The synthesis methods, catalyst performance, stability, and durability were examined. Key factors influencing performance, including metal species, nitrogen doping levels, support materials, and structural effects, are discussed. The review also addresses the challenges and future perspectives of p-block single metal site catalysts, aiming to guide future research and development in fuel cell technology.

Keywords: Oxygen Reduction Reaction (ORR), P-Block Elements, Single-Atom Catalysts, Fuel Cell Technology, Nitrogen-Doped Carbon

OP-037

Investigation of Binding Materials for Detaching TiO₂ Nanotubes for Enhanced Photoelectrochemical Applications

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Abstract

The efficiency of TiO₂ nanotubes (NTs) in photoelectrochemical (PEC) applications is often compromised by the inherent oxide layer formed on Ti films. To address this, our research focuses on the preparation and detachment of TiO₂ NTs from Ti films and their subsequent attachment to fluorine-doped tin oxide (FTO) substrates using various binding materials. TiO₂ NTs were synthesized through an anodization process and then detached using a second anodization method. The binding materials investigated in this study include TiO₂ nanoparticles (NPs), molybdenum carbide (Mo₂C), polyethylene glycol (PEG), and Nafion. The primary objective is to identify the most effective binding material that enhances the adhesion and electrical connectivity between the detached TiO₂ NTs and the FTO substrate, thereby improving PEC performance. The structural and morphological characteristics of the bound TiO₂ NTs were analyzed using scanning electron microscopy (SEM) and X-ray diffraction (XRD). Electrochemical impedance spectroscopy (EIS) and photocurrent measurements were conducted to evaluate the PEC efficiency. Preliminary results indicate that the choice of binding material significantly impacts the overall performance, with certain materials offering superior adhesion and reduced charge recombination. This study provides critical insights into optimizing the interface between TiO₂ NTs and FTO, paving the way for more efficient PEC devices.

Keywords: TiO₂ nanotubes (NTs); photoelectrochemical (PEC); Molybdenum carbide (Mo₂C)

OP-041

Performance Evaluation of a Lab-Scaled Anion Exchange Membrane Water Electrolyzer Under Varying Operating Parameters

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Abstract

Anion Exchange Membrane Water Electrolysis (AEMWE) offers a promising pathway for hydrogen production. Nevertheless, low energy efficiency and limited durability hinder its practical application. To address these limitations, a comprehensive understand of the factors influencing AEMWE performance is essential. This study focuses on the preliminary investigation of key operating parameters to assess their impact on hydrogen production and provide insights for future optimization efforts. A single-cell electrolyzer was employed to systematically evaluate the influence of feed temperature 30-60°C, 0.248-0.4612 mA/cm² and cell voltage 0.17 – 2.36 V start the reaction on the hydrogen production rate. The experimental setup include a 1 M KOH electrolyte circulated at 50 mL/min by a peristaltic pump through the anode side, with the electrolysis system operating at room temperature and atmospheric pressure, while voltage, current, hydrogen flow rate, and temperature were recorded every minute by an automatic data logger. Hydrogen production rate was monitored under varying conditions. Results indicate that an optimal combination of feed temperature of 58°C, current of 11.73 A and voltage of 2.21 V yield an average hydrogen production rate of 261 mL/min. These findings provide preliminary insights into AEMWE performance and serve as a basis for future optimization studies.

Keywords: anion exchange membrane (AEM) electrolyzer

OP-042

Enhanced Hydrogen Generation via Photoelectrochemical Water Splitting Using Kenaf-based Carbon Quantum Dots Modified BiVO₄

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Abstract

Bismuth vanadate (BiVO₄), a metal oxide with a favourable band edge position, is an excellent visible light photocatalyst for photoelectrochemical hydrogen production. However, its practical applications for hydrogen production are limited, wherein BiVO₄ photoanode has poor solar energy conversion efficiency due to its fast electron-hole recombination. Herein, a green approach using different loading amounts of kenaf-based carbon quantum dots (CQDs) as electron transfer mediators has been proposed to enhance the optical and electrical properties of the BiVO₄ photoanode. As compared with pure BiVO₄ photoanode, CQDs boosted the light absorption of the modified BiVO₄ photoanode across 300–800 nm and narrowed the band gap energy from 2.35 eV to 2.27 eV. In addition, the as-developed CQDs/BiVO₄ exhibited higher charge separation efficiency, with a 36.0% reduction in charge recombination at 469 nm. At 1.05 V vs. RHE, the optimum CQDs/BiVO₄ (CB-14) demonstrated a photocurrent density of 0.254 mA cm⁻², approximately two-fold compared to the unmodified BiVO₄. It also exhibited a 162% increment in photoconversion efficiency upon modification with kenaf-based CQDs. An average hydrogen evolution of 10.83 μmol cm⁻² h⁻¹ was recorded by CB-14, which is 1.67 times higher compared to the unmodified BiVO₄. The profound performance observed is attributed to the excellent electron transfer and sunlight harvesting ability of kenaf CDQs. This work demonstrates the potential of kenaf-based CQDs to enhance photoanode performance for green hydrogen evolution.

Keywords: photoelectrochemical; hydrogen production; BiVO₄; carbon quantum dots; kenaf

OP-043

Correlating Chemical Degradation and Ageing Phenomenon in Polymer Electrolyte Membrane (PEM) Water Electrolysis: A Bayesian Modelling Approach

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Abstract

Hydrogen production via Polymer Electrolyte Membrane (PEM) electrolysis is vital for the sustainable energy transition due to its high efficiency and generation of high-purity hydrogen. However, the durability and efficiency of PEM systems are challenged by degradation mechanisms such as gas crossover, chemical degradation, and membrane aging, which pose significant safety concerns regarding hydrogen storage and handling. Gas crossover occurs when hydrogen leaks through the membrane to the anode side, often due to membrane degradation. This leakage not only reduces current efficiency and increases energy consumption, as indicated by voltage readings, but also raises the risk of hazardous situations if hydrogen accumulates in unintended areas. Monitoring current efficiency can help identify gas crossover, while a sudden increase in voltage without a corresponding rise in current typically signals an efficiency problem linked to this issue. This paper presents a study on these degradation mechanisms and their correlations with aging phenomena in PEM electrolysis using Bayesian modelling, which incorporates electrochemical reactions and mass transport. Bayesian modelling effectively predicts membrane lifetime, providing a more efficient alternative to real-time studies, which are often costly and time-consuming. Additionally, it offers valuable insights for optimizing parameter settings. These advancements are crucial for enhancing the reliability and safety of PEM technology in the renewable energy sector, ultimately contributing to the development of safer and more efficient hydrogen production systems.

Keywords: *Polymer Electrolyte Membrane (PEM) electrolysis; hydrogen production; chemical degradation; Bayesian modelling; renewable energy*

OP-046

Preparation of a Carbon Nanofiber Layer for Electrode Support in Direct Methanol Fuel Cell with Taguchi Method

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Abstract

Direct methanol Fuel Cell (DMFC) performance depends on variable parameters that influence the electrode preparation processes. Nano-materials has attracted research community to adopted it in order to improve performance capability of fuel cell. Its unique structure to support the deficiency of commercial material is a great potential. Up to now, common electrodes in direct methanol fuel cell (DMFC) are carbon-based. The aim of this study was to develop and optimize a carbon nanofiber (CNF) anode electrode for a DMFC by using design of experiment (DOE). This study adopted the L_{16} orthogonal array (OA) Taguchi method to determine the optimal combination of factors. Variables, such as catalyst loading, catalyst support, nafion solution and fuel concentration, were analyzed so that the optimum parameters were selected according to the signal-to-noise ratio and an analysis of variance. In this study, each variable showed a significant effect on the cell performance. The half cell consisted of a nanofiber electrode for the anode side in contact with a solution that was developed using the optimal parameters obtained. The results showed a current density of 600 mAcm^{-2} . This study shows that the CNF electrode produces the highest current density compared to carbon black (CB). In addition, some physical analysis, including scanning electron microscopy, energy dispersive spectroscopy being conducted to study the evaluation of the nano-electrode structural to serve as better electrode.

Keywords: *Electrode; Direct Methanol Fuel Cell; Carbon Nanofiber Layer; Taguchi Method; Design of Experiment*

OP-047

Influence of Ni Loading on H₂ Selectivity and Production in the Dry Reforming of Methane Using Ultrasound-Assisted Ni/CeO₂ Catalysts

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Abstract

The pursuit of optimizing hydrogen production has driven research in heterogeneous catalysis for dry reforming of methane. Mesoporous nanocrystalline Ni/CeO₂ catalysts with varying nickel loadings were synthesized using ultrasonic-assisted citrate complexation and evaluated for the dry reforming of methane (DRM). Characterization through XRD and BET analysis revealed that increasing Ni loading from 1.5 wt.% to 12 wt.% significantly enhanced surface area from 17.67 to 39.43 m²/g, though further increase to 15 wt.% reduced it to 34.17 m²/g. Higher Ni loadings also led to smaller crystallite sizes and better dispersion. FESEM and TEM morphology analysis highlighted the crucial role of the ultrasonic-assisted method in producing small, uniform nano catalysts creating coral like shape. The catalyst with 12 wt.% Ni demonstrated superior performance in DRM, achieving hydrogen selectivity of 54% and hydrogen yield of 49% after 5 hours of reaction. These findings highlight the importance of optimizing nickel loading to develop high-performance DRM catalysts which are crucial for boosting hydrogen production and supporting today's energy transition agenda.

Keywords: dry reforming of methane, nickel, ceria, hydrogen yield

OP-050

Crystal Structure, Hirshfeld Surface Analysis and Energy Framework Calculations of N-(1,3-benzothiazol-2-yl)-R-benzamide (R-BZBA)

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Abstract

In the title compound, the x-ray crystal structure has been examined for structure optimization and quantum chemical analysis. Three crystal structures of benzothiazole were investigated. The effect of CF₃ substitution in ortho, meta and para position of N-(1,3-benzothiazol-2-yl)-R-benzamide (R-BZBA) in solid state arrangement was studied. Noncovalent bonding interactions were found to influence the arrangement of crystals in the solid-state structure. The crystal adopts a dimeric structure due to intermolecular N–H...N hydrogen bond interaction. Additionally, a delocalized C–F... π interaction was also reported as well as C–F...H and π ... π stacking interaction. Hirshfeld surface analysis, 3D fingerprints plot of interaction and the energy framework analysis were used to evaluate the interaction with the packing of the title compound using Crystal Explorer software.

Keywords: benzothiazole; Crystal Explorer; Hirshfeld surface; energy framework

OP-053

One-pot synthesis of MoS₂/Ni₃S₂/Ni Foam for Photoelectrochemical Hydrogen Production

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Abstract

With increasing global demand for fuel and electricity, coupled with the environmental challenges posed by greenhouse gas emissions from traditional energy sources, hydrogen fuel cell technology emerges as a promising alternative. Photoelectrochemical (PEC) water splitting, which utilises light as a primary energy source without combustion, is a viable method for sustainable hydrogen production. This study explores the potential of MoS₂/Ni foam as a photoelectrode for PEC applications. The MoS₂/Ni foam was synthesised via a one-pot hydrothermal method at 200°C, with varied hydrothermal durations. Morphological and elemental analyses were conducted using field emission scanning electron microscopy (FESEM) and energy-dispersive X-ray spectroscopy (EDS). X-ray diffraction (XRD) analysis confirmed the in-situ formation of Ni₃S₂ at 21.7°, 31.1°, 37.8°, 49.7°, 50.1°, and 55.1°, and MoS₂ at 14.4° and 38.1°. The results demonstrate that a 24-hour synthesis at 200°C yields a more well-defined crystalline phase than a 12-hour synthesis, highlighting the material's potential as a photoelectrode in PEC water splitting for green hydrogen production.

Keywords: Photoelectrochemical; Ni₃S₂ ; MoS₂ ; Hydrothermal



OP-060

Development of Efficient Z-Scheme Water Splitting Using $(W_{2/3}Y_{1/3})_2AlC$ as H_2 Evolution Photocatalyst and Pt-BiVO₄

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Abstract

Z-scheme systems have garnered significant attention for their ability to achieve overall water splitting through the utilisation of narrow-band-gap photocatalysts. To enhance the efficiency of these systems, it is imperative to improve the intrinsic activities of both the hydrogen evolution photocatalyst (HER) and the oxygen evolution photocatalyst (OER), facilitate effective electron transfer from the OER to the HER, and mitigate any back reactions that may occur. In this study, we have developed a high-performance photocatalyst, specifically $(W_{2/3}Y_{1/3})_2AlC$, to serve as the HER in a Z-scheme overall water splitting system, which is paired with Pt-BiVO₄ as the OER. By implementing surface modifications to enhance charge separation and redox reactions, this system can split water into hydrogen and oxygen for more than 720 hours, achieving a solar-to-hydrogen energy conversion efficiency of 0.31%. Remarkably, the water-splitting activity of this system shows only a minimal decrease when the background pressure is elevated to 210 kPa, a feature that contrasts with many existing photocatalytic systems. These findings indicate that the present system possesses characteristics well-suited for application under practical operating conditions.

Keywords: HER; OER; water-splitting; photocatalyst; Z-scheme

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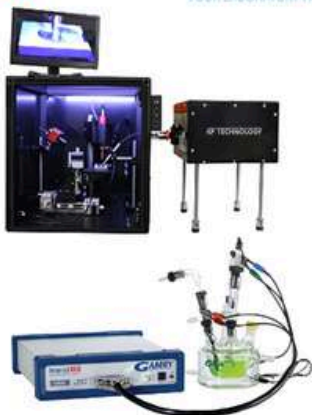
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