Exploration for New Catalysts Dedicated to a Green Environment

While challenging, research for promising catalysts using effective methods has an immense impact on the environment.

Human activities and the burning of fossil fuels result in carbon emissions, which release significant greenhouse gases that lead to global warming. Achieving carbon neutrality is critical in combating the climate crisis. Dr Bolong HUANG, Associate Professor of Department of Applied Biology and Chemical Technology at the Hong Kong Polytechnic University (PolyU), is dedicated to research in catalysis for the development of new catalyst materials that support sustainable energy supply and conversion technologies, aligning with the global vision of protecting the environment.

PolyU Highly Cited Researchers

Dr Bolong HUANG
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Highly Cited Researcher:
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Clarivate Analytics

Ever since the discovery of catalysts 200 years ago, they have become a significant area of research in modern times due to their ability to alter reaction path and accelerate the reaction with lower activation energy towards desired products. Even small quantities of catalysts can have a significant impact. Nowadays, catalysts are indispensable in over 90% of the chemical industry, influencing every aspect of our lives, including oil refining, plastics production, fertiliser manufacturing, medicine development, and energy supply.

Advanced cross-disciplinary research

Research in catalysis spans multiple disciplines, encompassing physics, chemistry, biology, and materials sciences. As catalysis involves both chemical reactions and physical processes, solid knowledge across scientific fields is pivotal for designing novel catalysts with high performance.

"My research satisfaction stems from the fact that my works can inspire more researchers and influential scientists in this field, in which all researches together accelerate the developments of advanced catalyst research for sustainable energy technologies."

In catalysis research, Dr HUANG has applied theoretical calculations and machine learning techniques to develop novel catalysts for important chemical reactions in sustainable development. These include water-splitting hydrogen (H_2) generation, oxygen reduction and evolution for fuel cells and metal-air batteries, and carbon dioxide (CO_2) reduction for controlling carbon emission.

Dr HUANG said, "My theoretical calculations not only accelerate the discovery of novel catalysts but also gain crucial insights into fundamental reaction mechanisms. I am driven to pursue catalysis research to identify more novel functional materials that can be applied in sustainable developments."

The quest for effective catalysts

Focusing on designing novel catalysts and investigating catalysis mechanisms for various chemical reactions, Dr HUANG's studies have garnered high citations worldwide, all driven by the ultimate goal of fostering a sustainable future.

Throughout the research journey, Dr HUANG said major challenges revolve around identifying the most suitable catalysts and developing effective methods. Due to the diverse range of catalysts in terms of morphologies, composition, activity, and stability, the quest for the most effective and robust catalyst for a specific application requires extensive efforts in the trial-and-error process.

By combining theoretical calculations and machine learning techniques, Dr HUANG's team accomplishes a comprehensive screening of single-atom catalysts across the periodic table. This approach allows them to identify the most suitable candidates to generate different high-value chemicals from CO_2.

The research titled "Accelerating atomic catalyst discovery by theoretical calculations-machine learning strategy" was published in ***Advanced Energy Materials*** in February 2020. The highly cited study presents crucial guidelines for experimental catalyst design and synthesis from two independent theoretical perspectives: density functional theory (DFT) and machine learning (ML) to achieve parallel explorations. The proposed advanced research strategy demonstrates the significant potential of atomic catalysts for efficient hydrogen generation.

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For research on CO_2 reduction reaction (CO_2RR) toward the generation of C_2 products (e.g. ethanol, ethylene, acetic acid), there has been the challenge of developing efficient and stable atomic catalysts to achieve high faradaic efficiency and selectivity, which are desirable for broad industrial applications due to their high value and energy density.

Dr HUANG's research, "Double-dependence correlations in graphdiyne-supported atomic catalysts to promote CO_2RR toward the Generation of C_2 Products," provides an advanced understanding of the complicated CO_2RR mechanisms, which is expected to aid the development of novel atomic catalysis for efficient C_2 products generation. The research was published in ***Advanced Energy Materials*** in December 2022. This highly cited work provides valuable insights and references for screening and predicting efficient atomic catalysts to overcome the current bottleneck in achieving efficient conversion from CO_2 to high-value-added C_2 products.

PolyU Highly Cited Researchers

Staying focused

Creating sustainable energy harvesting and conversion systems is crucial in addressing both the energy crisis and pollution caused by the use of fossil fuels. To achieve this, novel catalysts have been developed to accelerate electrochemical reactions such as hydrogen evolution and oxygen evolution/reduction reactions for sustainable energy systems such as fuel cells and water-electrolyser. Meanwhile, applying advanced catalysts in CO_2RR systems also supplies promising solutions for reducing carbon emissions towards carbon neutrality. Therefore, developing advanced and efficient catalysts are still one of the most important research topics for sustainable energy technologies.

Dr HUANG said, "A highly cited researcher must have an unwavering focus on the core interest and devote great efforts to solve key challenges in related fields." Despite encountering numerous ups

and downs throughout the research journey, Dr HUANG acknowledges these experiences and inspiration are critical for reaching impactful and meaningful research outputs in the future.

Looking ahead, Dr HUANG is committed to leveraging his expertise and experiences in theoretical calculations to design more advanced catalysts. The ultimate goal is to contribute to the advancement of technology for sustainable development.

Research Interests

Theoretical calculations of electronic structures on nanomaterials, energy materials, solid functional materials, and rare earth materials, as well as their applications in multi-scale energy conversion and supply systems.

Selected Highly Cited Publications

1. B. Huang, M. Sun, H. H. Wong, T. Wu, et. al., Double-dependence Correlations in Graphdiyne-supported Atomic Catalysts to Promote CO_2RR towards the Generation of C_2 Products, Advanced Energy Materials, 13, 2023.
2. B. Huang, M. Sun, H. H. Wong, T. Wu, et. al., Stepping Out of Transition Metals: Activating the Dual Atomic Catalyst through Main Group Elements, Advanced Energy Materials, 11, 2021.
3. B. Huang, M. Sun, A. W. Dougherty, Y. Li, et. al., Accelerating the atomic catalyst discovery by theoretical calculations-machine learning strategy, Advanced Energy Materials, 10, 2020.