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Nanocatalysis—facing a sustainable future

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Catalysis is at the heart of industrial processes, with an estimated 85–90% of manufacturing involving at least one catalytic step. From food products to everyday items like contact lens cleaners and detergents, catalysis is essential. Catalytic processes contribute to over 35% of global GDP, particularly in the petroleum, energy, chemicals, and food production industries.[1] As the global population grows and energy demands surge—projected to reach 29.5 billion TOE by 2100—catalysis will play an ever-greater role in meeting these challenges sustainably.

However, economic growth cannot come at the cost of increasing environmental pressures.[2] Hence, the need for advanced catalytic technologies that can support sustainable development is becoming urgent. The efficiency of catalytic processes depends on many factors, with structural and electronic properties of catalysts being central to their performance.[3] The rise of nanocatalysis, enabled by advances in nanoscience and nanotechnology, allows precise control over the composition, morphology, and electronic states of catalysts, greatly enhancing their functionality. Machine learning, advanced characterization techniques, and computational chemistry have all accelerated progress in this field, leading to remarkable breakthroughs.

This themed collection on nanocatalysis brings together a collection of articles that showcase cutting-edge developments and challenges in the field. The research spans a wide range of topics, including novel catalyst design, mechanistic insights, and catalytic applications across electrocatalysis, photocatalysis, and biocatalysis. Below is a brief overview of the articles featured in this collection, classified into five broad categories: design, structure, and mechanism of nanocatalysts; nanomaterials for electrocatalysis; nanomaterials for photocatalysis and photoelectrochemical application; nanomaterials for thermal catalysis; and emerging applications of nanocatalysts.

Rational design and mechanistic insights into high-performance nanocatalysts are key to developing more efficient catalysts. Tsukuda *et al.* (**https://doi.org/10.1039/D3NR05857C**) review recent advances in the synthesis and catalytic applications of atomically precise Au/Ag nanoclusters doped with single atoms, offering future perspectives on the rational development of active and selective metal nanocluster catalysts. Hsu *et al.* (**https://doi.org/10.1039/D4NR01178C**) systematically review advanced nanoscale catalysts for hydrogen production *via* water splitting, highlighting modification strategies such as doping, morphology control, and heterojunction/homojunction structures, along with the corresponding catalytic mechanisms. Heteroatom doping and interface engineering are effective strategies for regulating the electronic structure of catalysts, thereby enhancing their catalytic performance. Liu *et al.* (**https://doi.org/10.1039/D4NR01010H**) developed a high-performance hydrogen evolution catalyst by incorporating Ru atoms into a nanosheet array. Single-atom catalysts have gained significant interest for their near-100% atomic utilization and uniformly distributed active sites. Their performance can be enhanced by optimizing the surrounding coordination environment (**https://doi.org/10.1039/D4NR00337C**, **https://doi.org/10.1039/D4NR02650K**, **https://doi.org/10.1039/D4NR01635A** and **https://doi.org/10.1039/D4NR01134A**). In particular, Zou *et al.* (**https://doi.org/10.1039/D4NR00077C**) developed a dual-atom catalyst that surpasses the performance of single-atom catalysts. Using two-dimensional materials with highly exposed surfaces as substrates is considered an effective strategy for constructing efficient catalysts (**https://doi.org/10.1039/D4NR01517G**, **https://doi.org/10.1039/D4NR01911C**, **https://doi.org/10.1039/D4NR01117A**, **https://doi.org/10.1039/D4NR01122H**, **https://doi.org/10.1039/D4NR01932F**, **https://doi.org/10.1039/D4NR01743A**, **https://doi.org/10.1039/D4NR01013B**, **https://doi.org/10.1039/D4NR01611D**, **https://doi.org/10.1039/D4NR01168F**, **https://doi.org/10.1039/D4NR01154F**, **https://doi.org/10.1039/D4NR01186D**, **https://doi.**

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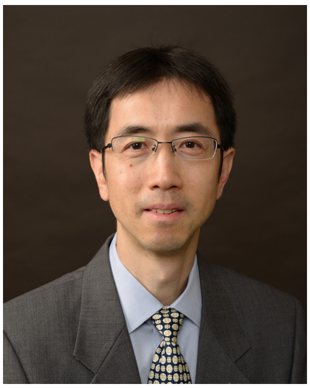
org/10.1039/D4NR00796D, https://doi.org/10.1039/D4NR01191K and https://doi.org/10.1039/D4NR00975D). In addition, high-entropy materials (https://doi.org/10.1039/D4NR00474D and https://doi.org/10.1039/D4NR01538J) offer significant advantages in catalysis due to their broader compositional design and flexible, diverse microstructures.

Regarding electrocatalysis, Wu *et al.* (https://doi.org/10.1039/D4NR02519A) developed intermetallic NiCo electrocatalysts to enhance the efficiency of the hydrogen evolution reaction in alkaline conditions. Wang *et al.* (https://doi.org/10.1039/D4NR01320D) employed an effective piezoelectric method to enhance catalytic water splitting activity significantly, without altering the material's morphology or composition, by modulating bulk charge separation. Yang *et al.* (https://doi.org/10.1039/D4NR01071J) enhanced hydrogen evolution efficiency by partially substituting nitrogen with oxygen in the Ni_3N catalyst, thereby tuning its electronic structure. In particular, Song *et al.* (https://doi.org/10.1039/D4NR00170B) accelerated the kinetically sluggish oxygen evolution reaction in water electrolysis by leveraging the photothermal effect. To enable overall water electrolysis for hydrogen production, Rajeshkhanna *et al.* (https://doi.org/10.1039/D4NR01196A) developed two non-precious metal materials, each designed to efficiently catalyze the hydrogen evolution and oxygen evolution reactions. Alongside water electrolysis for hydrogen production, CO_2 reduction is considered a promising method for decarbonization and sustainable energy conversion. This



Zhiqun Lin

Zhiqun Lin is currently a professor of chemical and biomolecular engineering at the National University of Singapore (NUS). He received his BS degree in materials chemistry from Xiamen University in 1995, his master's degree in macromolecular science from Fudan University in 1998, and his PhD degree in polymer science and engineering from University of Massachusetts, Amherst in 2002. He did his postdoctoral research at the University of Illinois at Urbana-Champaign. He joined the Department of Materials Science and Engineering at the Iowa State University as an assistant professor in 2004 and was promoted to associate professor in 2010. He moved to the Georgia Institute of Technology in 2011 and became a professor in 2014. He relocated to National University of Singapore in 2022. His research interests include photocatalysis, electrocatalysis, batteries, solar cells, block copolymers, conjugated polymers, functional nanocrystals, hierarchically structured and assembled materials, and surface and interfacial properties.

In Young Kim

In Young Kim is an assistant professor in the Department of Chemistry and Nanoscience at Ewha Womans University (EWU). She earned her PhD (2014) under the supervision of Prof. Seong-Ju Hwang at EWU. After completing her PhD, she worked as a postdoctoral fellow under the guidance of Prof. Ajayan Vinu at the University of South Australia (UniSA). In 2017, she was awarded the prestigious ARC DECRA fellowship, which marked the beginning of her independent research career at UniSA and The University of Newcastle. In 2020, she was appointed as an assistant professor at Chonnam National University before joining EWU in 2022. Her research expertise includes the development of 2D inorganic nanosheet-based nanohybrid materials and porous materials for energy and environmental applications. She is also highly skilled in analysing the local atomic structure of nanostructured materials using XANES/EXAFS techniques.

Michelle Personick

Michelle Personick is an associate professor in the Department of Chemistry at the University of Virginia (UVA). She received her BA from Middlebury College (2009) and her PhD from Northwestern University working with Prof. Chad Mirkin (2013). From 2013–2015, she was a postdoctoral researcher at Harvard University with Prof. Cynthia Friend and co-advised by Prof. Robert Madix. She began her independent career at Wesleyan University in 2015 before moving to UVA in 2023. Her current research includes the development of in situ *electroanalytical methods for understanding and designing materials syntheses as well as the application of precision nanomaterials in catalysis.*

themed collection highlights the development of novel nanocatalysts for efficient CO_2 electroreduction (https://doi.org/10.1039/D4NR01416B, https://doi.org/10.1039/D4NR01484G, https://doi.org/10.1039/D4NR01173B, https://doi.org/10.1039/D4NR00909F, https://doi.org/10.1039/D4NR00340C and https://doi.org/10.1039/D4NR01082E). The development of efficient oxygen reduction electrocatalysts contributes to advancing energy sustainability (https://doi.org/10.1039/D3NR06647A and https://doi.org/10.1039/D4NR02425G). The electrochemical reduction of nitrate to ammonia is a promising catalytic pathway for both ammonia production and nitrate reuse from industrial wastewater (https://doi.org/10.1039/D4NR01625D).

In the field of photocatalysis and photoelectrochemical applications, Waclawik *et al.* (https://doi.org/10.1039/D4NR00885E) review light modulation techniques to improve product selectivity in photocatalytic reactions. Yang *et al.* (https://doi.org/10.1039/D4NR01040J) discuss advancements in utilizing quantum dots for hydrogen production. Additionally, Seh *et al.* (https://doi.org/10.1039/D4NR02342K) highlight recent developments in photocatalysts, emphasizing strategies to enhance their performance in environmental remediation and energy conversion. Aizenberg and van der Hoeven *et al.* (https://doi.org/10.1039/D4NR01200C) discovered that the placement of nanoparticles in gold-loaded titanium dioxide (Au/TiO_2) inverse opals influences both photocatalytic activity and stability. Efficient hydrogen production and ammonia generation can be achieved by adjusting the structure (https://doi.org/10.1039/D4NR01194E) and electronic state (https://doi.org/10.1039/D4NR01787K and https://doi.org/10.1039/D4NR00868E) of the photocatalyst. In addition, constructing photocatalysts with porous frameworks is an effective strategy for enhancing photocatalytic efficiency (https://doi.org/10.1039/D4NR00779D, https://doi.org/10.1039/D4NR00608A and https://doi.org/10.1039/D4NR00391H). The development of efficient catalysts is also essential for photoelectrochemical applications (https://doi.org/10.1039/D4NR00949E).

In addition to electrocatalysis and photocatalysis, this themed collection also encompasses research on thermal catalysis. Frenkel *et al.* (https://doi.org/10.1039/D4NR01396D) identify the origins of reaction-driven aggregation and fragmentation of atomically dispersed Pt catalysts on ceria supports during the high-temperature water gas shift reaction. Machida *et al.* (https://doi.org/10.1039/D4NR01156B) found that the nanoscale smoothness of the Pt capping layer increases the TOF more than tenfold compared to a rough Pt surface in the ammonia oxidation reaction. Pomposo *et al.* (https://doi.org/10.1039/D4NR01261E) developed hetero-bimetallic single-chain nanoparticles as soft nanocatalysts, facilitating one-pot alkyne semihydrogenation and olefin double oxidation reactions in *N*-butylpyrrolidone at room temperature, without the need for toxic solvents like *N*,*N*-dimethylformamide. The study by Behrens *et al.* (https://doi.org/10.1039/D4NR02025A) demonstrated that Ni,Fe catalysts supported on zirconia and ceria exhibited higher activity than those on magnesia in CO_2 hydrogenation, attributed to changes in metal–support interactions resulting from differences in reducibility and oxygen vacancy formation. Nanomaterials derived from metal–organic frameworks are also regarded as an effective strategy for developing efficient catalysts (https://doi.org/10.1039/D4NR01185F). Additionally, constructing composite nanocatalysts can effectively enhance catalytic activity, selectivity, and stability (https://doi.org/10.1039/D4NR01184H, https://doi.org/10.1039/D4NR01211A, https://doi.org/10.1039/D4NR01222D, https://doi.org/10.1039/D4NR01116C, https://doi.org/10.1039/D4NR01409J, https://doi.org/10.1039/D4NR00948G, https://doi.org/10.1039/D4NR01243G, https://doi.org/10.1039/D4NR00358F and https://doi.org/10.1039/D3NR06518A).

Finally, this themed collection highlights emerging applications of nanocatalysis in biocatalysis, biosensing, and batteries. Negishi *et al.* (https://doi.org/10.1039/D4NR02506G) report the design and construction of a novel (3,6)-connected two-dimensional silver cluster-assembled material, used for the first time as a support matrix for enzyme immobilization. Tong *et al.* (https://doi.org/10.1039/D4NR01208A) reveal the unique pH-dependent behaviors of iron oxide nanozymes and ascorbic acid, paving the way for macrophage-based cell therapy. Wang *et al.* (https://doi.org/10.1039/D4NR00521J) developed a nanoengineering approach for highly sensitive vanillin detection using neodymium niobate nanospheres on functionalized carbon nanofibers. In addition, developing efficient catalysts for both the cathode and anode can significantly enhance overall battery performance (https://doi.org/10.1039/D4NR00518J, https://doi.org/10.1039/D4NR02385D and https://doi.org/10.1039/D4NR02418D).

This themed collection represents the diverse, interdisciplinary nature of nanocatalysis research, from theoretical insights to practical applications in energy, sustainability, and health. We hope the collection provides readers with a comprehensive overview of recent progress and future directions in nanocatalysis. We extend our thanks to all contributing authors, reviewers, and the editorial and production staff for their support in bringing this themed collection to fruition.

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