Materials Horizons

EDITORIAL

Cite this: DOI: 10.1039/d6mh90024k

Introduction to the themed collection on nanocatalysis

Huabin Zhang, *[a] Jennifer Strunk, [b] Marcella Lusardi,*[c] Tianyi Ma, [d] Vivek Polshettiwar *[e] and Wee-Jun Ong *[f]

DOI: 10.1039/d6mh90024k

rsc.li/materials-horizons

The field of catalysis stands at a pivotal juncture. As societies worldwide grapple with the twin imperatives of sustainability and decarbonisation—from clean energy to carbon recycling, from environmental remediation to sustainable chemical manufacturing—the design of catalysts that are efficient, selective, stable, and scalable has never been more urgent. In this context, the cross-journal themed collection "Nanocatalysis" in *Nanoscale Horizons* and *Materials Horizons* offers a timely, high-impact platform for showcasing cutting-edge research at the interface of nanoscience, materials design, and catalysis.

Why nanocatalysis now?

Nanostructured catalysts bring unique and transformative advantages over their bulk counterparts. Through precise control of particle size, crystal facets, surface structure, and hierarchical assembly, nanocatalysts can dramatically enhance active site dispersion, optimise reactant diffusion pathways, and modulate electronic environments. Such engineered control enables unprecedented catalytic activity and selectivity. As highlighted in the collection's introduction, this control underpins progress in diverse, societally critical areas, ranging from solar-driven water splitting and CO_2 conversion to environmental remediation and sustainable chemical synthesis.

Beyond structural miniaturisation, nanocatalysis is increasingly defined by *function-driven design*. Concepts such as defect engineering, interface-dominated reactivity, electronic and spin effects, light–matter interactions, and dynamic restructuring under reaction conditions are reshaping how catalytic performance is understood and optimised. These advances signal a shift from empirical optimisation toward mechanism-informed, physics-guided catalyst design, positioning nanocatalysis as a foundational discipline rather than a niche subfield of catalysis.

Moreover, the versatility of nanoscale materials—encompassing metals, metal oxides, MOFs, composites, doped nanostructures, heterojunctions, and hybrid systems—makes nanocatalysis a unifying framework that connects energy, environment, materials, and chemical sectors. At a time when global challenges demand cross-disciplinary solutions, nanocatalysis exemplifies the power and necessity of this integration.

Purpose and scope of the collection

The "Nanocatalysis" collection was conceived to provide a comprehensive, curated snapshot of where the field stands, where it is headed, and what challenges remain. Guest Edited by an international team with wide-ranging expertise, the collection brings together fundamental studies, methodological advances, mechanistic insights, and emerging applications.

The scope is deliberately broad, capturing the design, synthesis, and characterization of nanostructured catalysts; computational and theoretical modelling of mechanisms; and innovative applications in energy (water splitting, CO_2 reduction), environmental remediation (pollutant degradation), and sustainable chemistry (valorisation, selective conversion). By doing so, the collection aims not only to highlight top-tier research but also to foster cross-fertilization between subfields that may traditionally have been siloed. The collection also serves as a bridge to connect fundamentals with applications, underscoring how control at the nanoscale serves as the foundation for efficient materials and process design across length scales in practice.

[a] *Center for Renewable Energy and Storage Technologies (CREST), Physical Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal 23955-6900, Kingdom of Saudi Arabia. E-mail: huabin.zhang@kaust.edu.sa*
[b] *Department of Chemistry, Technical University of Munich, Lichtenbergstraße 4, Garching near Munich D-85748, Germany*
[c] *Princeton Materials Institute, Princeton University, Princeton, NJ, 08544, USA. E-mail: mlusardi@princeton.edu*
[d] *School of Science, Royal Melbourne Institute of Technology University, Melbourne, VIC 3000, Australia*
[e] *Department of Chemical Sciences, Tata Institute of Fundamental Research, Mumbai, 400005, India. E-mail: vivekpol@tifr.res.in*
[f] *Center of Excellence for NaNo Energy & Catalysis Technology (CONNECT), School of Energy and Chemical Engineering, Xiamen University Malaysia, Sepang, Selangor Darul Ehsan 43900, Malaysia. E-mail: weejun.ong@xmu.edu.my*

Highlights: sampling some of the exciting contributions

Within this rich tapestry of work, several contributions already stand out for their originality, ambition, and potential impact. A recent review on MOF-based and derivative catalysts for photoelectrocatalytic water splitting (https://doi.org/10.1039/D5MH01457C) provides a comprehensive and critical analysis of how modular MOF architectures can be transformed into highly efficient photoelectrocatalytic systems, highlighting challenges such as charge separation and long-term stability. Complementing this, advances in phosphite-incorporated, surface-confined cobalt electrocatalysts (https://doi.org/10.1039/D5TA05452D) demonstrate how nanoscale active-site engineering can significantly enhance hydrogen evolution activity. Equally compelling is the work on asymmetrically tipped MoS_2/CdS heterojunction photocatalysts (https://doi.org/10.1039/D5MH00658A), which achieve high-performance photoreforming of plastic waste into hydrogen, underscoring the potential of nanocatalysis to address both energy generation and waste valorisation. From a mechanistic perspective, studies revealing how spin-polarised Fe-TAML complexes can tune oxygen-reduction selectivity illustrate the profound impact of electronic structure control on catalytic pathways (https://doi.org/10.1039/D5MH00615E). Together, these papers exemplify the diversity, creativity, and conceptual advances characterising this themed collection.

Significance for the community and future directions

By gathering these works under a single ''Nanocatalysis'' umbrella, the collection offers more than the sum of its parts. It provides a curated lens through which researchers across academia and industry can take stock of the field's current frontiers. For newcomers, the collection presents a guided entry; for experts, it highlights gaps, challenges, and emerging opportunities.

In particular, the collection underscores the critical role of interfacial design, structural control, mechanistic understanding, and hybrid material strategies—themes increasingly recognised as essential for next-generation catalytic systems. It also reveals the growing convergence of catalysis with allied disciplines: nanomaterials, photonics, electrochemistry, environmental science, waste valorisation, and renewable energy. Underpinning these ties is the governing role that electronic structure plays on function, and the way such structure is achieved, characterized, and controlled to unlock unprecedented performance across such diverse application domains.

Importantly, the collection also highlights a broader evolution in the field: from isolated performance metrics toward holistic evaluation of catalytic systems. Increasing attention is being paid to stability, *operando* behaviour, scalability, and integration with realistic reaction environments. Such perspectives are essential if nanoscale discoveries are to mature into deployable technologies, reinforcing the role of nanocatalysis as a bridge between fundamental insight and societal impact.

Looking forward, we anticipate that future work will deepen mechanistic understanding (*e.g. via in situ*/*operando* techniques, advanced computational modelling), expand materials diversity (2D materials, single-atom catalysts, metal–organic frameworks, high entropy materials, heterostructures), and push toward system-level integration (*e.g.* combining catalysis with separation, reactor design, life-cycle analysis). We also expect growth in translational research, where insights from nanoscale design feed into scalable, real-world applications, including sustainable chemical manufacturing, energy storage and conversion, environmental remediation, and circular economies.

The ''Nanocatalysis'' collection in the context of the *Horizons*' mission

The ethos of *Nanoscale Horizons* and *Materials Horizons* has always been to publish work that offers a conceptual advance, promoting new ways of thinking about nanoscience, nanotechnology and materials science. This collection exemplifies that ethos: by focusing on nanocatalysis, it challenges and expands traditional boundaries of catalysis research, embedding it within a nanoscience framework. It builds bridges: between disciplines, between fundamental and applied science, between academic research and practical challenges. In doing so, the ''Nanocatalysis'' collection positions itself as a milestone—not only for the journals, but for the broader catalysis, materials, and nanoscience communities.

Conclusion

In a time when the world demands sustainable solutions to energy, environment, and materials challenges, the ''Nanocatalysis'' collection emerges as a showcase of innovation, creativity, and ambition at the nanoscale. It celebrates recent achievements, stimulates critical reflection, and invites the community to contribute further.

We hope that this collection will inspire new collaborations, seed fresh ideas, and accelerate progress toward catalytic systems that are efficient, sustainable, and transformative.

As the field continues to mature, nanocatalysis will play a central role in redefining how catalysts are conceived, evaluated, and ultimately implemented—anchored in nanoscale control, but guided by system-level thinking.

Huabin Zhang

Huabin Zhang is an associate professor at King Abdullah University of Science and Technology (KAUST). He received his PhD from the Chinese Academy of Sciences in 2013 and subsequently conducted postdoctoral research at the National Institute for Materials Science (NIMS), Japan, followed by a Research Fellow position at Nanyang Technological University (NTU), Singapore. He joined KAUST as an assistant professor in 2021 and was promoted to associate professor in 2025. His research focuses on the atomic-level design of catalysts for photo- and electrocatalysis. Zhang has published over 170 SCI-indexed papers, receiving more than 22 000 citations with an H-index of 76. He has been named a Clarivate Highly Cited Researcher consecutively from 2021 to 2025 and currently serves as an associate editor on Science Advances.

Jennifer Strunk

Jennifer Strunk is a full professor in industrial chemistry and heterogeneous catalysis at the Technical University of Munich, Germany. She received her diploma and PhD in industrial chemistry from the Ruhr-University Bochum. After a postdoctoral stay at UC Berkeley, she became junior research group leader at Ruhr-University in 2010 and in 2014 independent group leader of the group Nanobased Heterogeneous Catalysis at the MPI for Chemical Energy Conversion. Since 2017 she has been an associate professor at Leibniz Institute for Catalysis at the University of Rostock, before joining TU Munich in 2023. Prof. Strunk conducts research in the fields of heterogeneous catalysis and photocatalysis. The goal is the activation of small stable molecules, such as the recycling of carbon dioxide into chemical production and the activation of nitrogen. In particular, the focus is on understanding the light- and heat-driven physical and chemical elementary steps to enable scaling up from the laboratory to industry.

Marcella Lusardi

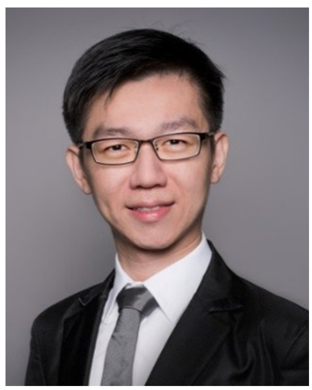
Marcella Lusardi is an assistant professor of chemical and biological engineering at the Materials Institute at Princeton University. Before joining Princeton, Lusardi was a research scientist at BASF. Lusardi's research centers on the design of advanced catalytic materials using new synthetic techniques that tailor material structure at the molecular level, integrating fundamental insights and impactful catalytic technology commercialization. Her work has been recognized with the ACS PRF Doctoral New Investigator Award.

Tianyi Ma

Tianyi Ma is a RMIT University Distinguished Professor, an Australian Research Council Future Fellow, Fellow of Royal Society of Chemistry, and Clarivate's Global Highly Cited Researcher. He is Director of ARC Industrial Transformation Hub for Intelligent Energy Efficiency in Future Protected Cropping (E2Crop), and Research Director of the Centre for Atomaterials and Nanomanufacturing (CAN). His international standing is evidenced by >500 publications in top-tier journals with an H-index of 113 and >53 000 citations. His ground-breaking research has been acknowledged by internationally recognised experts and authorities via the 2024 Prime Minister's Prize for Science – the Malcolm McIntosh Prize for Physical Scientist of the Year, AAS Le Févre Medal, and Young Tall Poppy Science Award.

Vivek Polshettiwar

Vivek Polshettiwar is a professor of chemistry at TIFR, Mumbai. The work of Polshettiwar in the nanocatalysis realm of "Black Gold" and "Defects" represents a quintessential example of how fundamental science can drive innovation. Their detailed exploration of plasmonic photocatalysis and defect engineering offers new perspectives on material design, catalysis, and sustainability, paving the way to explore the vast potential of nanomaterials in solving environmental and energy challenges. He is a recipient of the ORISE Research Fellowship (US-EPA), the Asian Rising Star Lectureship at the 15th Asian Chemical Congress (awarded by Nobel Laureate Ei-ichi Negishi), the CRSI Bronze Medal, and the MRSI Medal. He is a Fellow of the National Academy of Sciences, India; the Indian Academy of Sciences; and the Royal Society of Chemistry (UK). His honors include the 2022 IUPAC-CHEMRAWN VII Prize for Green Chemistry, the Falling Walls Winner (Physical Sciences, 2023), and the 2024 Shanti Swarup Bhatnagar Award, India's highest science honor, conferred by the President of India.



Wee-Jun Ong

*Wee-Jun Ong is a professor and Assistant Dean in the School of Energy and Chemical Engineering at Xiamen University Malaysia. He received his BEng and PhD in chemical engineering from Monash University. Starting in 2021, he serves as the Director of the Center of Excellence for NaNo Energy & Catalysis Technology (CONNECT). Since September 2024, he has been an adjunct professor of the College of Engineering at Korea University. Previously, he was a scientist at the Agency for Science, Technology and Research (A*STAR), Singapore. In 2019, he was a visiting professor at Technische Universität Dresden and Lawrence Berkeley National Laboratory. His research interests include nanomaterials for photo(electro)catalytic and electrochemical H_2O splitting, CO_2 reduction, H_2O_2 production, plastic upcycling, nitrate reduction, urea synthesis, and biomass valorization, as well as microwave plasma methane cracking. To date, he has published more than 170 SCI-indexed papers with total citations of over 27 000 and an H-index of 75. He has been named a Clarivate Highly Cited Researcher from 2019 to 2025. He currently serves as an Associate Editor of SmartMat and has been appointed to the Advisory Boards of several leading journals such as Materials Horizons, Journal of Materials Chemistry A, Small, and Nano Research.*

