

Harnessing natural minerals for sustainable electrocatalysis

Zhijie Chen^{1,*} and Bing-Jie Ni^{1,*}

¹Water Research Centre, School of Civil and Environmental Engineering, The University of New South Wales, Kensington, NSW 2052, Australia

*Correspondence: zhijie.chen1@unsw.edu.au (Z.C.); bingjie.ni1@unsw.edu.au (B.N.)

Received: September 25, 2025; Accepted: November 21, 2025; Published Online: November 22, 2025; <https://doi.org/10.59717/j.xinn-mater.2025.100176>

© 2025 The Author(s). This is an open access article under the CC BY license (<https://creativecommons.org/licenses/by/4.0/>).

Citation: Chen Z. and Ni B. (2025). Harnessing natural minerals for sustainable electrocatalysis. *The Innovation Materials* 3:100176.

Electrocatalysis, powered by renewable electricity, offers a scalable and environmentally benign platform to drive sustainable energy and environmental systems (e.g., water splitting, CO₂ reduction, nitrogen fixation, pollutant remediation) with high selectivity and minimal emissions. Yet the viability of electrocatalysis at scale ultimately depends on the development of catalysts that are not only active and durable but also economically and environmentally sustainable. Currently, most state-of-the-art electrocatalysts are derived from precious metals such as platinum (Pt), iridium (Ir), and ruthenium (Ru). While these materials deliver high activity and stability, their scarcity and prohibitive cost severely constrain large-scale deployment.¹ Moreover, many advanced nanostructured catalysts rely on complex designs and multi-step syntheses, such as high-temperature annealing or chemical vapor deposition, which increase carbon footprints and compromise sustainability goals. These limitations highlight the urgent need for alternative catalyst platforms that are abundant, cost-effective, and environmentally compatible.

Natural minerals, formed through geological processes, represent one such alternative. Composed of earth-abundant elements such as iron, nickel, cobalt, manganese, and molybdenum, minerals feature diverse coordination environments, multiple oxidation states, and well-defined crystal structures that provide intrinsic catalytic functionality.² Transition metal sulfides, such as molybdenite (MoS₂), and oxides, such as pyrolusite (β-MnO₂), are emblematic cases where redox-active sites and favorable electronic structures enable electrocatalytic activity. Beyond direct utilization, minerals can be modified to enhance performance or serve as conceptual blueprints for the rational design of next-generation catalysts. Therefore, leveraging natural minerals through direct utilization, targeted modification, and mineral-inspired engineering presents a transformative opportunity to build a

genuinely sustainable platform for electrocatalyst development.

DIRECT UTILIZATION: FROM ROCKS TO CATALYSTS

The most straightforward strategy is the direct use of natural minerals as electrocatalysts. This “short-process” approach leverages natural abundance while avoiding the energy- and carbon-intensive steps associated with conventional catalyst synthesis (Figure 1A). Molybdenite (MoS₂), has been widely reported as an efficient catalyst for hydrogen evolution reaction (HER), highlighting how raw minerals can rival synthetic materials in performance. Similarly, naturally occurring Fe and Ni-based sulfide minerals can be directly ground into powders and used as catalytic electrodes, bypassing costly purification or complex synthesis.

Direct utilization has three key advantages: simplicity, scalability, and cost-effectiveness. Yet challenges remain. Most minerals suffer from limited surface area, poor electronic conductivity, and compositional heterogeneity, which restrict activity and reproducibility compared with noble-metal benchmarks. Overcoming these barriers requires both systematic mapping of mineral resources and complementary modification strategies.

MODIFICATION: UNLOCKING HIDDEN POTENTIAL

To unlock the full catalytic potential of minerals, tailored modification strategies are often indispensable. Physical, chemical, and structural treatments can dramatically improve their intrinsic activity, stability, and adaptability for diverse catalytic reactions. Mechanical activation (e.g., high-energy milling or grinding) can reduce particle size, induce amorphization, create structural defects, and expose unsaturated metal sites, thereby enhancing surface reactivity and enriching active sites.² Extraction-post-treatment, in

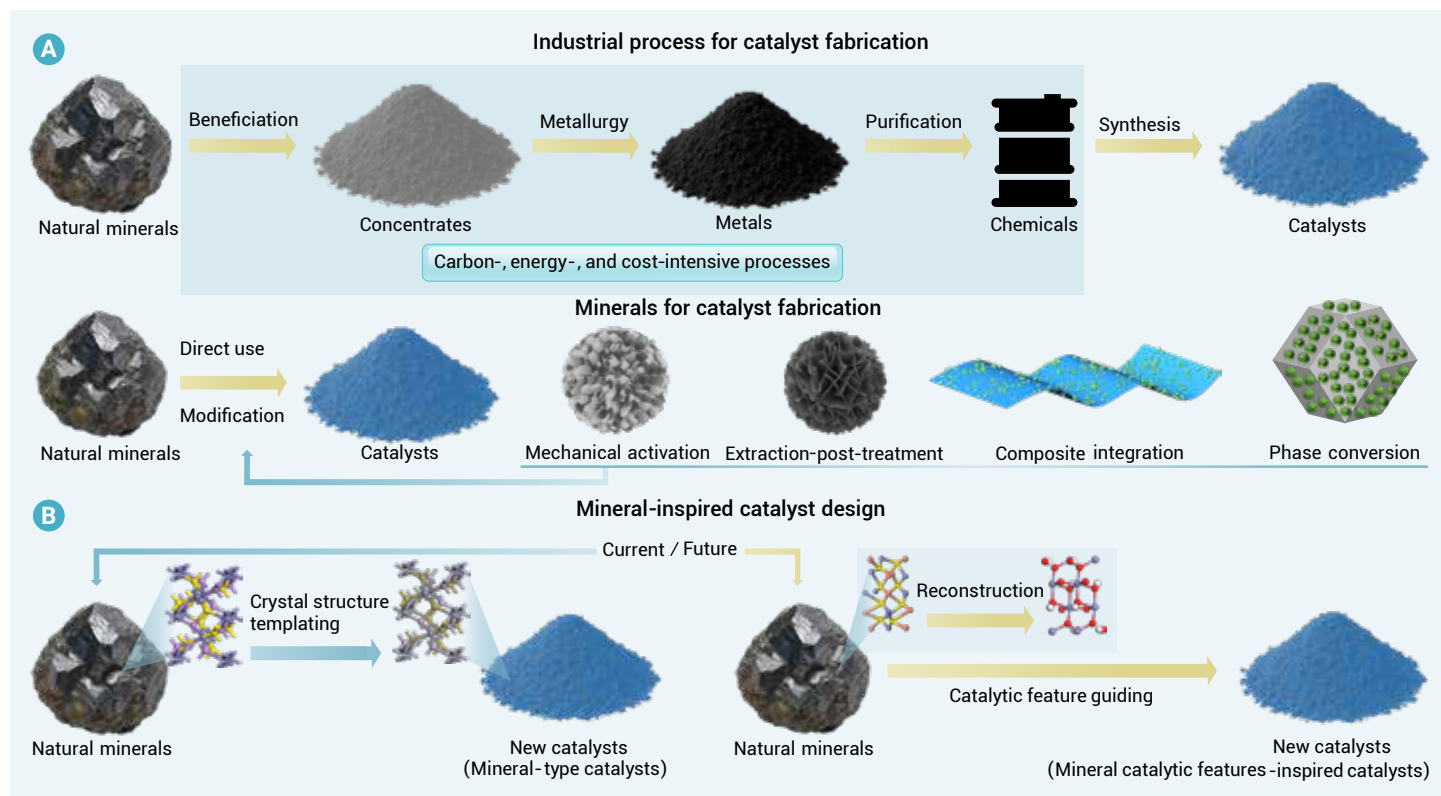


Figure 1. Natural minerals for electrocatalyst development (A) Comparison of current industrial process for catalyst fabrication and mineral-based catalyst fabrication. (B) Development of mineral-inspired catalyst design.

which functional components are selectively extracted from minerals and subsequently modified, enables the synthesis of predesigned catalysts with optimized composition and functionality. Using a chloride-mediated diffusion strategy, Zhang et al. synthesized dual-atom catalysts comprising Fe–Mg atomic pairs from unrefined natural ores. The adjacent Fe and Mg atoms exhibited a unique synergistic interaction, leading to significantly enhanced performance in electrocatalytic CO₂ reduction.³ Composite integration further expands versatility by coupling minerals with conductive frameworks such as carbon nanotubes, graphene, or electroactive species (e.g., atomically dispersed metals), thereby improving charge transport, structural robustness, and active site accessibility. For example, the molybdenite-derived MoS₂/Mo₂C hybrid has shown superior HER performance compared with many noble-metal catalysts, owing to accelerated electron transfer and synergistic interfacial coupling.⁴ Phase conversion strategies also play a crucial role, transforming minerals into heterostructural catalysts or new phases with emergent properties through controlled sulfidation, oxidation, or reduction.

The sustainability of modification approaches is critical. Overly energy-intensive processes risk negating the low-carbon advantages of mineral-based catalysis. Future efforts should therefore prioritize green modification pathways that minimize energy input, reduce chemical waste, and employ environmentally benign conditions. Examples include mechanochemical activation, which eliminates the need for solvents and high temperatures; low-temperature or ultrafast treatments, which drastically cut energy consumption; and bio-assisted processes, which operate under mild, aqueous conditions with minimal chemical additives. By aligning performance enhancement with low-energy, low-impact processing, modified minerals can evolve from geological curiosities into truly sustainable and practical electrocatalyst platforms.

MINERAL-INSPIRED ENGINEERING: BEYOND STRUCTURES TO CATALYTIC FEATURES

The most transformative strategy, mineral-inspired engineering, reimagines minerals as conceptual blueprints for designing advanced electrocatalysts. Traditionally, this approach has focused on structure-inspired design (Figure 1B), replicating static mineral features like crystal lattices, multi-anion compositions, or multi-metallic coordination to generate “mineral-type” catalysts.⁵ For example, pyrite (FeS₂) has served as a model for developing transition metal sulfides active in HER, oxygen evolution reaction (OER), and oxygen reduction reaction.¹

What is largely missing, however, is a catalytic features-inspired perspective. Generally, minerals in electrochemical processes will undergo dynamic transformations such as surface reconstruction, oxygen mobility, ion exchange, and interfacial buffering. These adaptive features are often the true origin of catalytic activity. For instance, sulfide minerals can transform under OER conditions into high-valent metal oxyhydroxides, which constitute the real active phase. Similarly, such restructuring can be accelerated by intrinsic characteristics of minerals, including low crystallinity and multivalent composition, creating highly active and self-renewing catalytic interfaces. These transformations are not parasitic degradation but self-adaptive evolutions that continuously regenerate the active surface. Understanding and harnessing such features through in situ/operando spectroscopy and theoretical modelling will be essential to translate mineral adaptability into the rational design of synthetic catalysts.² Insights gained from minerals with clear crystal structures and physicochemical features can be distilled into transferable catalytic features and reaction characteristics, providing valuable lessons for new catalyst design, offering pathways to exploit mineral templates more rationally and efficiently while avoiding the long, labor-intensive trial-and-error cycles of traditional catalyst development.

Positioning mineral-inspired engineering in this way reframes the field: from copying mineral structures to learning from mineral catalysis. Few studies to date have taken this step, but doing so could unlock a fundamentally new design paradigm. Embedding insights from mineral catalytic features, including dynamic restructuring, oxygen mobility, ion-exchange adaptability, and interfacial buffering, into synthetic materials can enable the creation of catalysts that are not only compositionally flexible but also functionally adaptive. In this sense, catalytic features-inspired catalyst design represents the most forward-looking frontier in minerals-based electrocatalysts, offering a powerful pathway to sustainable catalysis.

Despite encouraging progress, minerals-based electrocatalysts remain at an early stage, and several directions demand urgent attention. First, the challenges of mineral heterogeneity and modest intrinsic activity must be addressed, but systematic cataloguing of mineral compositions and the development of scalable, green modification strategies could transform variability into opportunity, particularly if mining tailings and industrial residues are explored as cost-effective catalyst feedstocks. Second, moving beyond structure mimicry toward catalytic behavior-inspired design represents the most transformative opportunity. Decoding adaptive processes such as surface reconstruction, ion exchange, and interfacial buffering through in situ/operando spectroscopy, theory, and artificial intelligence (AI)-driven screening could establish new descriptors that transcend conventional models. Third, practical progress requires system-level integration, where mineral-based catalysts advance beyond proof-of-concept studies and into real devices, including electrolyzers, CO₂ capture–conversion systems, and water treatment modules.

Building on these priorities, a structured technical roadmap is essential for translating mineral-based catalyst concepts into scalable technologies. A feasible pathway could involve: (i) material discovery, guided by mineral databases and in silico screening to identify promising mineral analogues; (ii) catalyst optimization, using low-energy modification or mineral catalytic behavior-inspired design to enhance performance; (iii) electrode and cell integration, where mineral-based catalysts are incorporated into scalable architectures such as flow-cell configurations; and (iv) system-level validation, combining experimental testing with AI-assisted performance prediction and techno-environmental assessment. Such a roadmap highlights iterative feedback between theory, synthesis, and system engineering, ensuring efficient translation from fundamental discovery to practical deployment.

Evaluating the environmental footprint of mineral-based catalysts through life-cycle assessment (LCA) will also be crucial to substantiate their sustainability potential. LCA can quantify the energy consumption, greenhouse gas emissions, and resource depletion across the entire catalyst lifecycle—from mineral extraction and modification to operation and recycling. Integrating LCA with techno-economic analysis (TEA) will provide a balanced understanding of performance gains and environmental trade-offs, guiding low-impact mineral sourcing and process design.

By reframing minerals not as passive geological curiosities but as dynamic frameworks for catalyst design, we can pioneer a new generation of electrocatalysts that are simultaneously active, durable, and sustainable. Realizing this vision will require concerted, interdisciplinary collaboration across geochemistry, electrochemistry, materials informatics, and sustainability science. Integrating mineralogical insights with advanced characterization, theoretical modelling, and LCA-informed design can accelerate progress from fundamental discovery to scalable application, ultimately reshaping not only how we design catalysts, but how we value Earth's resources in the era of sustainable technology.

REFERENCES

- Gao M.-R., Zheng Y.-R., Jiang J., et al. (2017). Pyrite-type nanomaterials for advanced electrocatalysis. *Acc. Chem. Res.* **50**:2194–2204. DOI:10.1021/acs.accounts.7b00187
- Chen Z., Zheng R., Wei W., et al. (2022). Unlocking the electrocatalytic activity of natural chalcopyrite using mechanochemistry. *J. Energy Chem.* **68**:275–283. DOI:10.1016/j.jechem.2021.11.005
- Zhang H., Yuan J., Chen Y., et al. (2025). From Earth-abundant mineral sources to high-efficiency dual-atom catalysts: A chloride-guided one-pot synthesis approach. *Small Methods Early View* e01259. DOI:10.1002/smt.202501259.
- Zhang C., Luo Y., Tan J., et al. (2020). High-throughput production of cheap mineral-based two-dimensional electrocatalysts for high-current-density hydrogen evolution. *Nat. Commun.* **11**:3724. DOI:10.1038/s41467-020-17121-8
- Zhang X.-L., Yu P.-C., Su X.-Z., et al. (2023). Efficient acidic hydrogen evolution in proton exchange membrane electrolyzers over a sulfur-doped marcasite-type electrocatalyst. *Sci. Adv.* **9**:eadh2885. DOI:10.1126/sciadv.adh2885

FUNDING AND ACKNOWLEDGMENTS

This work was financially supported by the Australian Research Council (ARC) Linkage Project (LP240100542). The funder had no role in study design, data collection and analysis, decision to publish, or preparation of the manuscript.

DECLARATION OF INTERESTS

The authors declare no competing interests.