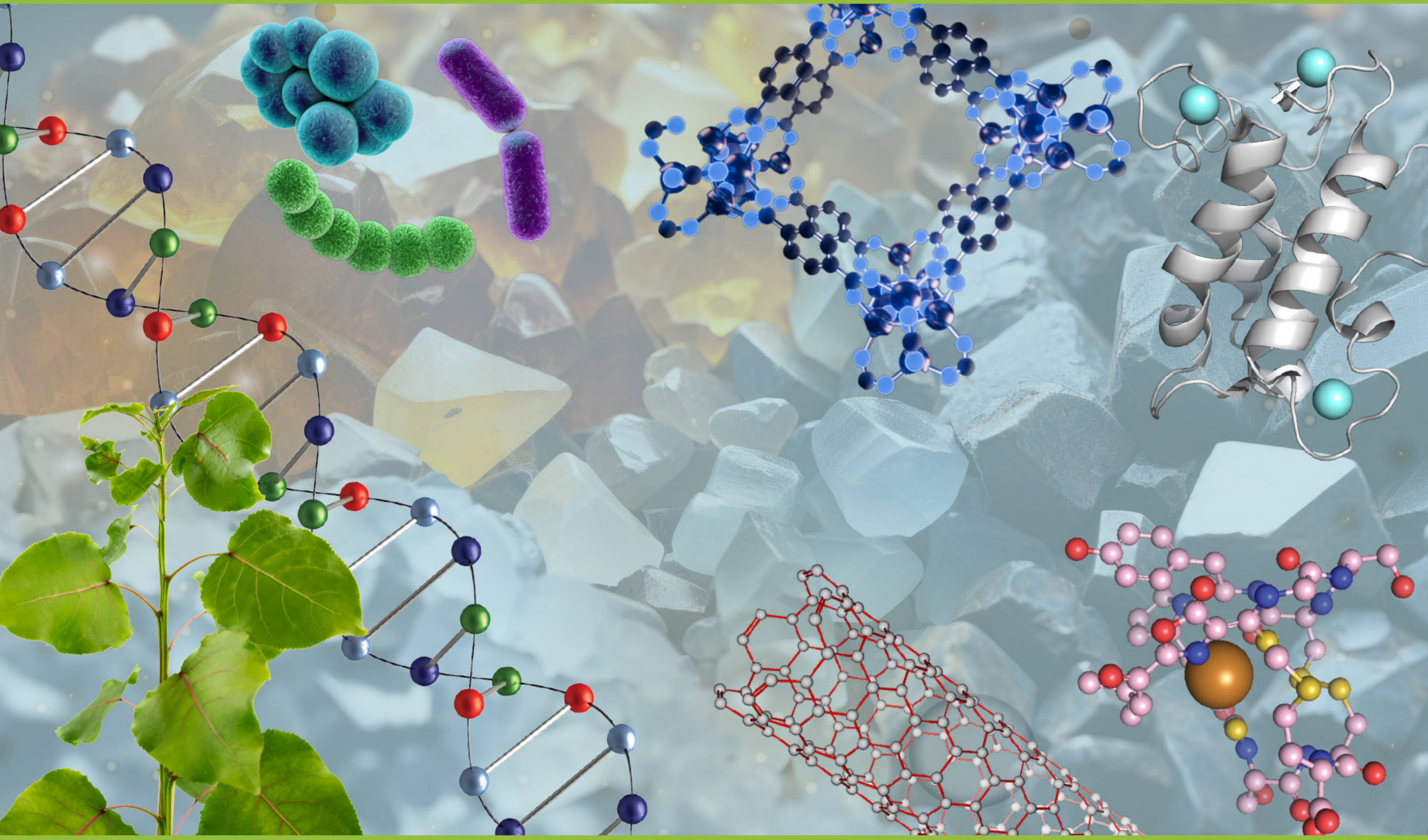
DOE/SC-2030

Basic Research Needs for

Biological Molecular Mechanisms for Critical Minerals and Materials

Integrative Biological, Chemical, and Materials Science Foundations for Securing Critical Minerals and Materials



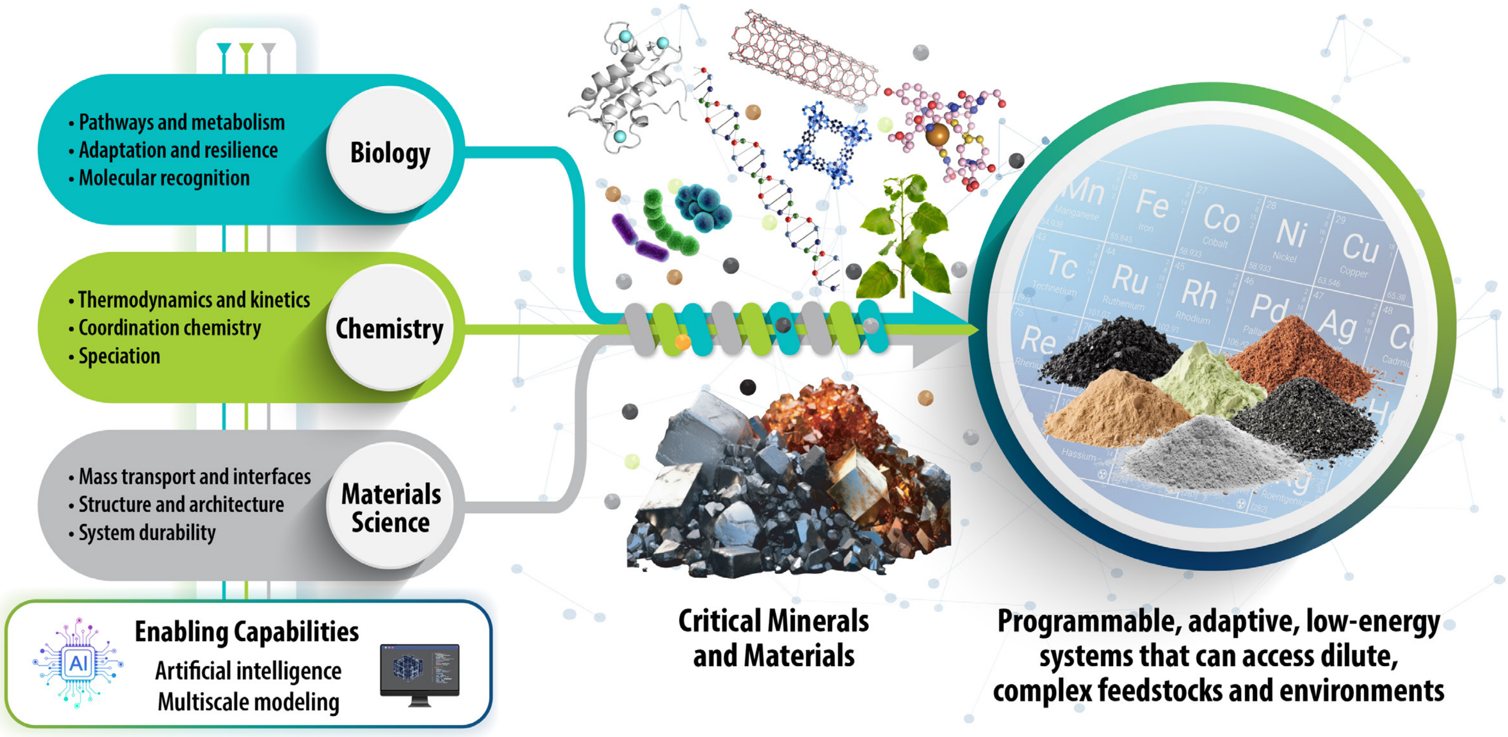
U.S. DEPARTMENT of ENERGY | Office of Science

From Molecules to Systems: Integrating Biology, Chemistry, and Materials Science for the Future of Critical Minerals and Materials

Critical minerals and materials (CMMs) underpin energy systems, advanced manufacturing, national defense, and emerging technologies, yet their supply chains are constrained by geological dispersion, geopolitics, and energy-intensive processing. Many CMMs are not rare but occur at low concentrations within complex ores and waste streams where conventional technologies optimized for high-grade ores become less efficient and economically viable. The convergence of biology, chemistry, and materials sciences offers innovations to dramatically enhance CMM recovery, transformation, and use.

Biology offers distinctive properties—molecular-scale selectivity, operation under ambient conditions, adaptability to complex and limiting environments, and opportunities for design of new functions—that could benefit CMM extraction and separation. Chemistry and materials sciences provide advantages of high-throughput, durability, and compatibility with industrial process infrastructure. Biological and chemical pathways could be exploited for not only extraction and separation but also exploration of functional substitutes for critical minerals. However, the basic principles governing biological–mineral–material interactions remain poorly understood, limiting predictive design and scalable deployment. Coordinated advances are needed to integrate molecular biology, biophysics, coordination chemistry, geochemistry, materials science, and multiscale modeling, coupled with AI-enabled discovery and experimentation.

In December 2025, the U.S. Department of Energy's (DOE) Office of Science (SC) convened a workshop to address Basic Research Needs for Biological Molecular Mechanisms for Critical Minerals and Materials. Co-sponsored by DOE SC programs in Basic Energy Sciences and Biological and Environmental Research, the workshop identified five priority research directions to establish scientific foundations for next-generation CMM recovery, separation, and substitution by integrating biology, chemistry, and materials sciences.



Integrated Biology, Chemistry, and Materials Science Enable New Frameworks for Critical Minerals and Materials (CMMs). Biology provides programmable recognition and adaptive pathways; chemistry defines coordination, kinetics, and energetics; and materials science facilitates transport, durability, and scalability. Together, they create bio-enabled and biohybrid pathways for selective, low-energy CMM discovery, recovery, separation, and substitution. AI and multiscale modeling link molecular interactions to system-level performance, enabling predictive design across scales.

Priority Research Directions

Determine compatibility of biotic and abiotic processes relevant to CMMs

Key Questions: *How can unconventional integration of biological, chemical, and materials processes enable new pathways for CMM recovery and separation, reducing unit operations or enabling co-production? What atomic, molecular, and systems-level drivers determine compatibility between biological and abiotic processes?*

Biological systems offer distinctive mechanisms for interacting with CMMs and possibilities for co-design with chemical separations and materials architectures to improve process efficiency. Research is needed to determine how biological systems can be modified to incorporate novel chemistries or embedded within, or coupled to, abiotic processes and materials (e.g., membranes, sorbents, and interfaces). Such design rules can reveal if processes can be integrated to reduce energy input, increase selectivity, and unlock new routes for complex and dilute CMM feedstocks.

Control dynamic interfacial processes and kinetics for CMM transformation

Key Question: *What molecular- and mesoscale interactions control the kinetics and mechanisms of CMM transformation at bio–mineral–material–fluid interfaces under realistic conditions?*

CMM transformation and recovery are governed by dynamic interfacial processes spanning biological systems, mineral surfaces, and engineered materials. In natural and biohybrid interfaces, these processes in part control mobilization rates, selectivity among competing ions, fouling or passivation behavior, and long-term system stability, yet predictive design rules are limited. Integrated in situ characterization, multiscale modeling, and AI tools are needed to connect molecular interactions to mesoscale transport and macroscale performance, enabling design of scalable CMM recovery systems.

Enhance CMM selectivity and reactivity for on-demand, low-energy-input pathways

Key Questions: *How can biological pathways or bioinspired analogs be designed to coordinate steps into stimulus-responsive systems that amplify selectivity and improve process efficiency? What design principles and synthetic methods can generate biological or biohybrid materials that simultaneously exhibit high selectivity, favorable kinetics, and durability?*

Biology achieves metal ion selectivity through coordinated pathways that integrate partially selective steps involving ligands, redox control, regulation, and spatial organization. CMM processing strategies could similarly leverage pathway-level control, thereby coordinating recognition, transport, transformation, and release while balancing selectivity, kinetics, reversibility, and durability. Biological, biohybrid, and bioinspired pathways can be programmed and controlled for selective, reversible, and energy-efficient CMM capture, transport, and release by integrating coordination chemistry, protein and peptide science, metabolomics, and materials design.

Predict systems resilience and adaptability in complex environments

Key Questions: *How do CMM-relevant biological, biohybrid, and bioinspired systems (e.g., molecules, organisms, and communities) persist and evolve in complex environments? How can experimental data and physics-based modeling across time and length scales be integrated to understand, discover, and improve biological, biohybrid, and bioinspired processes and to create predictive models for CMM recovery?*

Biological systems exhibit resilience and adaptability in heterogeneous and dynamic environments characteristic of many CMM feedstocks. There is a lack of predictive understanding of how these properties emerge from the interplay of molecular-scale processes, cellular regulation, and community dynamics. Biohybrid systems introduce additional constraints. Integrated experimental–theoretical and AI approaches are needed to uncover general principles of resilience. Such principles can enable rational design of adaptive biological and biohybrid CMM recovery systems that maintain performance under real-world conditions.

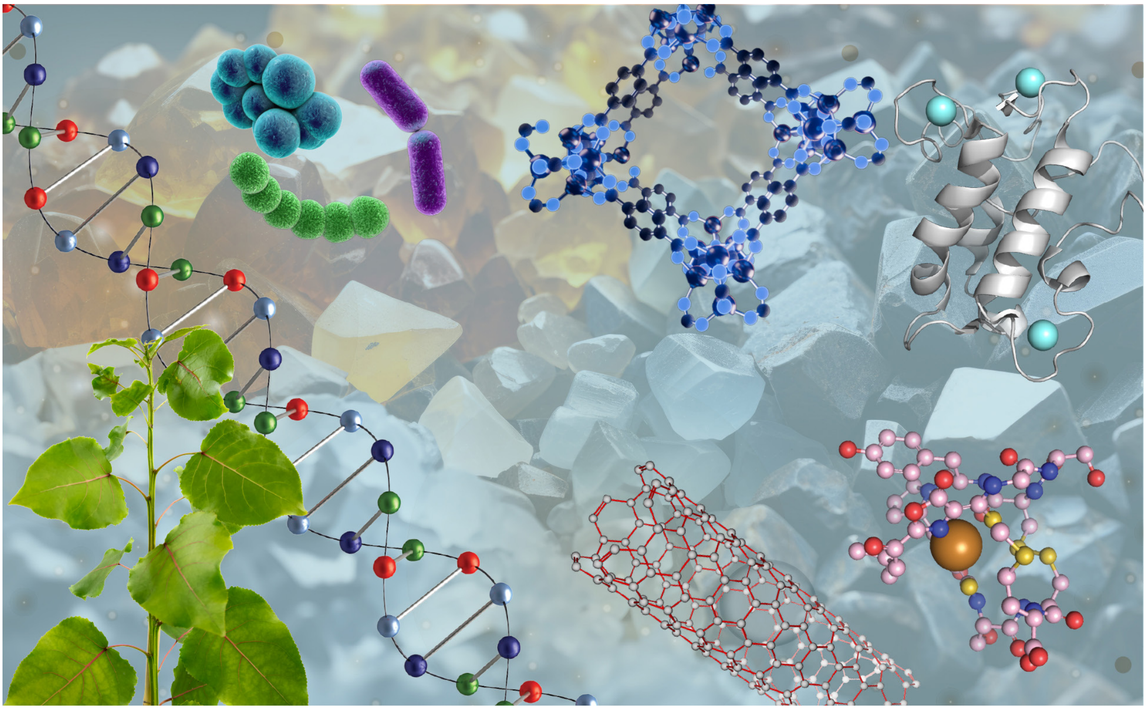
Design biological or bioinspired processes that minimize the need for CMMs

Key Questions: *What biophysical and chemical design principles enable biological or biohybrid systems to deliver robust, durable performance under conditions typically requiring inorganic CMMs? How do biological systems achieve comparable functions using abundant elements, hierarchical organization, and dynamic regulation?*

Critical minerals are valued for the functions they enable. In nature, shifts in metal availability often drive alternative biological strategies through natural selection for achieving similar biochemical functions. A knowledge gap lies in identifying which CMM functions can be substituted directly by biological or biohybrid architectures, and which may be surpassed by biology-enabled or bioinspired designs. Integrating molecular biophysics, coordination chemistry, materials science, and systems biology can enable design that transcends specific elements, reducing reliance on CMMs and producing materials that leverage biological adaptability, efficiency, and resilience.

Summary

Advancing innovative CMM recovery pathways requires a shift in the study, design, and integration of biological, chemical, and material processes. The priority research directions identified here move beyond sequential, energy-intensive extraction and separation toward integrated, adaptive, and low-energy systems capable of operating on chemically complex and dilute feedstocks. Challenges include establishing molecular-level understanding of CMM interactions at bio–mineral–material–fluid interfaces; elucidating the kinetic, thermodynamic, and transport processes that govern selectivity, durability, and system evolution; and developing predictive models that link molecular recognition to system-level performance. Progress will require advances in multiscale characterization; precision engineering of biological and biohybrid systems; and theory-driven, data-enabled modeling. Equally critical is defining the principles that govern resilience, adaptability, and durability of biological and biohybrid systems under dynamic conditions. Finally, biological and chemical insights can inspire component design that reduces or eliminates reliance on costly CMMs for function.



https://doi.org/10.2172/3028739

U.S. DEPARTMENT of ENERGY | Office of Science