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A “Reactivity-First” Framework for Critical Minerals: Molecular Speciation to Process-Scale Outcomes

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Critical minerals (CMs) are often evaluated through inventories (grade, tonnage, bulk assays), yet supply-chain resilience is frequently constrained by a deeper issue: we under-resolve CMs reactivity that governs recoverability, losses to waste streams, and environmental mobility. I propose a reactivity-first, multimodal workflow that links molecular-scale mechanisms to process-scale outcomes across the CMs supply chain, illustrated with vanadium (V), lithium (Li), molybdenum (Mo), and tungsten (W).

The workflow is organized around decision points that translate directly to extraction and circularity: (i) host-phase and micro-heterogeneity mapping to determine where CMs reside and how textures constrain accessibility; (ii) molecular speciation to define reactive pools and transformation pathways; (iii) interface process mapping under realistic fluids to quantify competitive sorption, ligand-promoted mobilization, and passivation; (iv) kinetics and transport constraints controlling rates, metastable intermediates, and scale-dependent behavior; and (v) scale transfer to unit operations (beneficiation, leaching, separation), tailings evolution, and end-of-life recycling. Li provides a deliberate counterpoint to V–Mo–W, requiring reactivity descriptors that remain valid across brines, clays, hard-rock silicates, and recycled feedstocks.

Central to this framework is explicit treatment of synergistic and competitive interactions among CMs and matrix components (Fe–Mn–Al phases, sulfides, carbonates, organics), which can amplify or suppress recovery and drive unintended co-mobilization. By integrating spectroscopy/microscopy, isotopic and solution tracers, controlled reactivity experiments, and geochemical/reactive-transport modeling, the proposed workflow yields mechanism-anchored descriptors that are portable across deposits, processing conditions, and circularity pathways, moving CMs characterization from “what is present” to “how it behaves.”