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AI-assisted mineral feedstock identification for integrating enhanced rock weathering (ERW) and geological hydrogen formation in closed engineered systems

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The co-production of hydrogen during alteration of $Fe^{(II)}$-bearing minerals offers a promising pathway for integrating enhanced rock weathering (ERW) with emerging geological hydrogen systems [2]. However, many prospective feedstocks, particularly basalts and other nominally Fe-rich lithologies, often exhibit lower reactivity in engineered settings than predicted from natural analogues, especially in closed configurations that impose mass-transfer and redox constraints [7]. This discrepancy highlights the need for predictive tools that identify mineral classes capable of rapid, near-complete reaction in closed ERW reactors, where hydrogen generation, alkalinity release, and mineral transformation must be precisely managed [6].

We present an AI-assisted workflow to evaluate and rank $Fe^{(II)}$-containing feedstocks for their potential to generate hydrogen and enhance silicate weathering under engineered, closed-system conditions. The workflow integrates targeted mineralogical and geochemical characterization, machine-learning models trained on datasets from serpentinization, iron oxidation, and radiolytic systems [2–4], and simulations predicting reaction completeness and gas yields. Because H_2 generation depends on the availability and oxidation state of $Fe^{(II)}$, quantifying $Fe^{(II)}/Fe^{(III)}$ ratios using Mössbauer spectroscopy or XANES is essential for predicting feedstock reactivity. Advanced spectroscopic approaches (Mössbauer, XANES/EXAFS) and microstructural imaging (SEM/TEM) further illuminate bonding environments and alteration textures that control dissolution rates and H_2 yield.

The workflow identifies cases where promising minerals nonetheless display sluggish or incomplete reaction pathways due to passivating alteration rinds, redox-limited kinetics, or restricted fluid access [3,4,6]. These insights guide the design of upcoming experiments in a prototype closed ERW reactor, where model outputs will be used to forecast feedstock performance and diagnose mechanistic bottlenecks that may suppress hydrogen generation or weathering rates [7]. Ultimately, this approach links engineered systems with natural analogues of hydrogen formation and migration, supporting improved strategies for selecting effective mineral feedstocks and advancing integrated ERW–geologic hydrogen technologies [1,2,5].

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