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Enabling AI in Reactive Transport Modeling with Community Data Mining

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Mineral–water interface processes are central to controlling the fate, transport, and bioavailability of metals in natural and engineered environments. Accurate prediction of metal adsorption and surface complexation is essential for understanding soil and groundwater metal mobility, optimizing industrial water treatment, designing resource recovery systems, and managing agricultural and mining impacts.

We are interested in transforming large, heterogeneous datasets of metal sorption and titration into robust, uncertainty-aware models that can be efficiently deployed in environmental and industrial simulations. The L-SCIE database and associated workflows (see https://github.com/mzavarin/L-SCIE) have shown promise in developing community data-driven surface complexation modeling framework to derive representative reaction chemistries on mineral surfaces (e.g. ferrihydrite, goethite, hematite, magnetite)—minerals ubiquitous in soils, sediments, and industrial systems. Recent additions to the database have led to a compilation of over 100,000 individual sorption data that are poised to open new approaches to data-driven modeling of interfacial reactions.

FAIR sorption databases, automated workflows, and surrogate modeling are poised to transform environmental and industrial modeling and assessment. We are developing a convergent strategy: (1) build FAIR, curated sorption and titration databases, (2) develop self-consistent surface complexation parameter frameworks constrained by community data, and (3) deploy hybrid physics–ML or GP surrogate approaches to efficiently and robustly propagate adsorption behavior into simulation and process design models. This same approach can be explored in the context of pore scale modeling, critical materials and metals extraction, and subsurface C cycling.