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A Chemistry Informed Hybrid Machine Learning Approach to Predict Metal-Mineral Surface Interactions

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Historically, reactive transport models have provided important simulation results on the mobility and fate of radionuclides in subsurface geologic systems. The effectiveness of these models hinges in part on surface complexation models (SCMs) that provide geochemically informed sorption-based retardation information. While our SCM reaction workflow using the recently developed Lawrence Livermore National Laboratory Surface Complexation/Ion Exchange (L-SCIE) database reasonably predicts uranium-quartz sorption for a large number of literature-mined data (n=526, R = 0.88-0.94, depending on the choice of SCM construct), a hybrid machine learning (ML) approach has shown promise in improving predictions (R^2 = 0.90-0.97). At its core, the random forest (RF) ML approach presented in this study is motivated by a successful effort in digitizing raw sorption community data from the RES^{3}T SC reaction constant database. Our new hybrid ML model incorporates important geochemical information through aqueous speciation calculations while also implementing a data-driven RF decision making process to calculate effects driven by mineral sorption phenomena. Named the LLNL Speciation Updated Random Forest (L-SURF) model, this high performing new hybrid approach is shown to have applicability to other radionuclide-mineral systems, as is demonstrated by the test case of uranium-montmorillonite sorption (n = 698, R^2 = 0.92-0.98). The approach can address various metal contaminant reactive transport modeling needs and may be applicable to both rock and mineral community sorption datasets.