Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.18842

Collective Solvent Dynamics in Model Geochemical Reactions

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Interactions between water and dissolved ions play a critical role in many geochemical processes. Water exchange reactions are intimately connected to mineral growth and dissolution rates, and solvent fluctuations can govern rates of charge transfer reactions in solution. I will discuss the non-trivial role of solvent effects in water exchange and redox reactions. To characterize the dynamics of these processes, we borrow and extend concepts from nonequilibrium physics and combine them with computer simulations to make predictions that connect with experimental data. I will first describe theories for the complex dynamics of exchange reactions involving ionic species, with a focus on understanding the scaling of exchange rates with ion-water interaction strength and ion concentration. Then, I will discuss applications of ideas from the physics of glassy systems to characterize electron transfer reactions in highly confined interlayers of layered oxides, where slow and collective solvent dynamics give rise to spatially heterogeneous reaction rates. These findings provide new insights into basic molecular-scale geochemical processes and illustrate how progess can be made by connecting with other disciplines.