Molecular Dynamic simulations of nanoconfined water in the clay matrix

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Fine-grained sedimentary rocks play an important role in a wide variety of modern energy technologies: from petroleum geology; geological carbon sequestration; to radioactive waste management. Yet, despite their utility and ubiquity, many of their properties remain poorly understood. In particular, the ability to predict the nanoscopic permeability of the clay matrix (often found within such fine-grained sedimentary rocks) remains one of the largest fundamental challenges in the geosciences, with potentially transformative implications.

In the present work, we show how large-scale classical molecular dynamics simulations can be used to help interpret the phenomenon of nanoscale diffusion and confinement of water and ions within the clay matrix. All-atom simulations containing multiple discrete clay particles are utilized to understand the roles of dry bulk density (porosity) and pore water chemistry on the microstructural, mechanical and transport properties of the clay matrix. Special emphasis is placed on comparing our results with available experimental data.