



Molecular Dynamics Can Predict Continuum-Scale Porous Media Properties

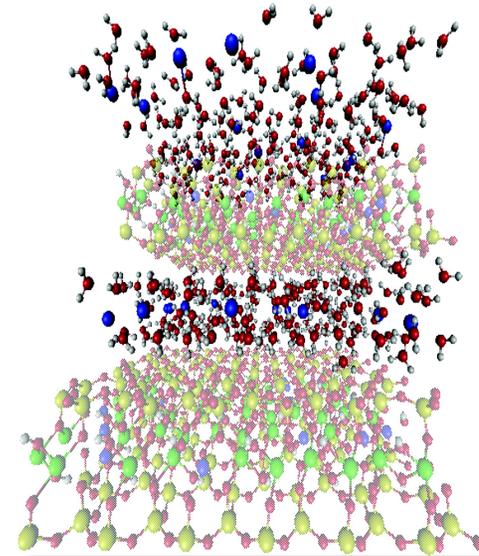
Objective: *Molecular-scale* understanding of chemistry and mass transport in nanoporous geologic media.

Implications: Nanoconfined water & solutes behave differently than their bulk liquid counterparts; difference may result in nanoporous media with remarkable properties for contaminant remediation, nanofluidics, and biotechnology.

- **Accomplishments:** Showed that molecular simulations at nanometer- and nanosecond-scale can help explain behavior of natural porous systems on scales of centimeters and days.
- Can accurately predict diffusion coefficients widely used in evaluating radioactive waste and CO₂ repositories.

NERSC: Used MOLDY code, 32 -64 cores on Bassi

I. Bourg, G. Sposito (LBNL)



Snapshot of the molecular dynamics simulation cell for the two-layer hydrate of Na-montmorillonite, with Na (blue), water O (red), and water H (white) atoms in the interlayer and Si (yellow), Al (green), Mg (blue), O (red), and H (white) atoms in a clay mineral structure.

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