Thematic Session 28

Multiscale computational modeling of clay-related materials and their fluid interfaces

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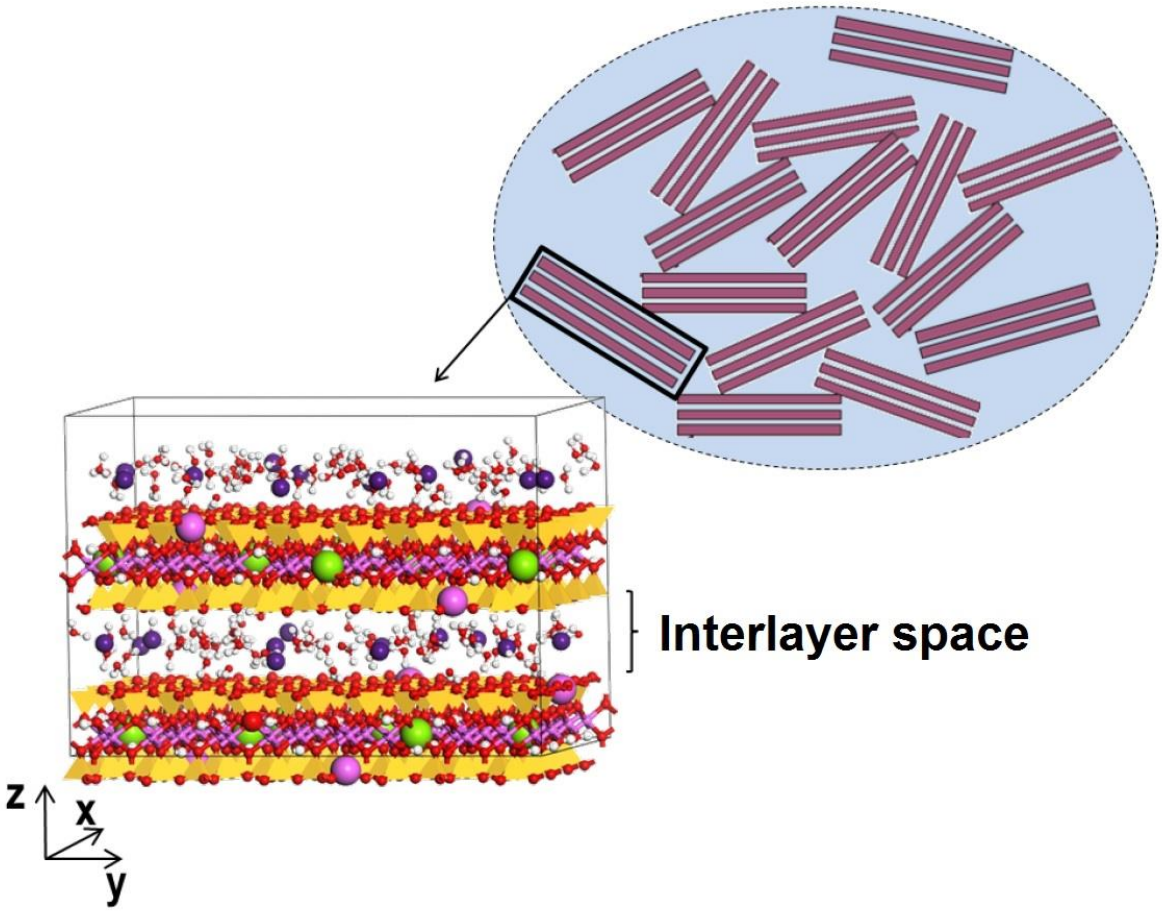
Clay-fluid interfaces are important in many natural and engineered processes controlling mineral weathering and dissolution, adsorption and release of contaminants in soil and water, long-term stability of geological nuclear waste repositories, exploitation of unconventional hydrocarbon sources, and geological carbon sequestration. Fundamental molecular-scale understanding of the chemistry and physics involved in all these processes is essential. Over the last 20 years, computational modeling techniques are increasingly applied in the clay research community to address these issues.

We invite contributions on all aspects of computer modeling of clays and their interfaces with aqueous and non-aqueous fluids using various computational techniques from quantum ab initio, to classical force field based molecular simulations, to mesoscale coarse-grained methods, etc. The contributions bridging different time and length scales and making direct links between computer simulations and molecular scale experimental studies, such as synchrotron X-ray, neutron scattering, and other advanced surface sensitive techniques are especially encouraged.

Keywords: Multiscale computer simulations, Molecular dynamics, Monte Carlo, Clay-fluid interfaces, Nano-confined fluids, Adsorption, Diffusion, Intercalation, Swelling.

Potential Journals: Clays and Clay Minerals, Applied Clay Science, Clay Minerals, Geochimica et Cosmochimica Acta, ACS Earth and Space Chemistry.


Interlayer space
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