

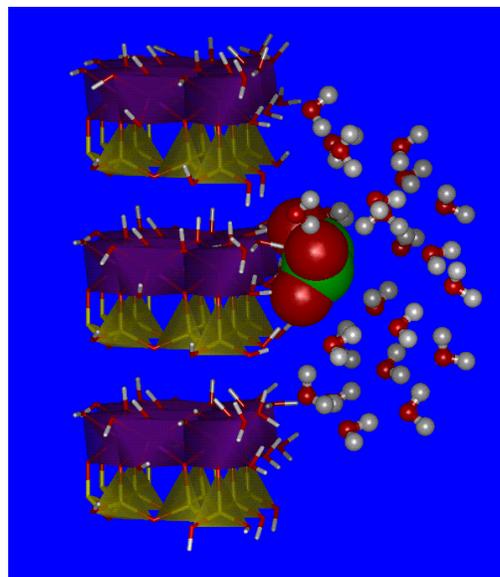


Atomistic and Molecular Simulations in Geochemistry and Materials Science

Description

Atomistic and molecular simulations of many geochemical and materials science processes are based on molecular mechanics and quantum-chemical calculations. Empirical methods utilize selected forcefields and can examine static and dynamic interactions of mineralogic and aqueous systems containing up to 5000 atoms when performed on modern workstations. *Ab initio* calculations, however, often require the use of more powerful computers to calculate both chemical reactions and electronic structures, especially for periodic systems. Simulation techniques include:

- Energy Minimizations
- Molecular Dynamics (MD)
- Ionic Modeling
- Monte Carlo
- Hartree Fock Molecular Orbital
- Local Density Functional Molecular Orbital



Sorption of Solvated Oxalate Anion onto (010) Edge Site of Kaolinite Clay

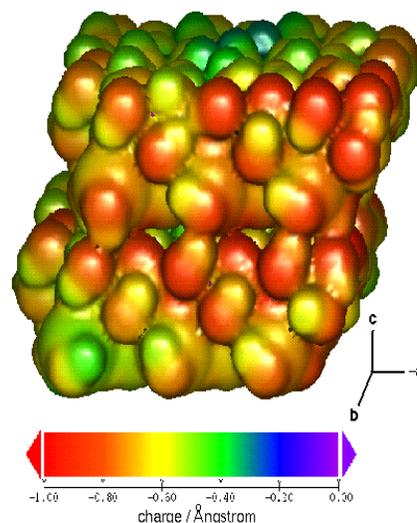
Needs

Geochemistry

- Bulk mineral structure refinement
- Characterization of surface relaxation
- Metal and organic ion sorption mechanisms
- Reactivity of mineral-solution interfaces
- Precipitation and dissolution reactions

Materials Science

- Sol-gel precursor conformations
- Ionic diffusion rates and mechanisms
- Ceramic growth morphology
- Substrate binding mechanisms



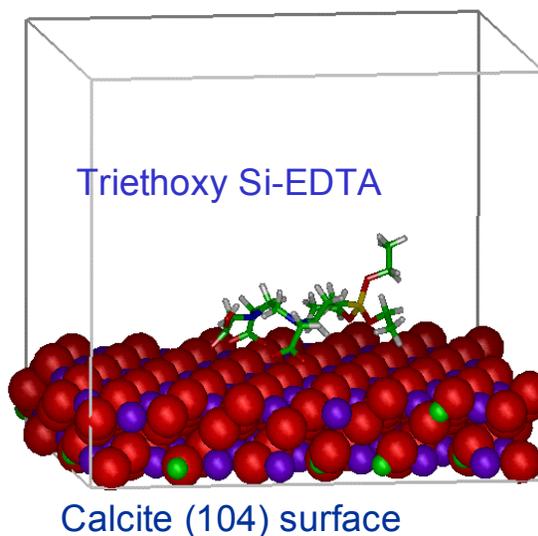
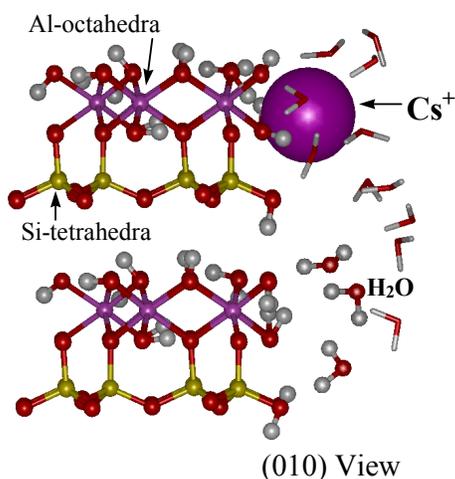
Molecular Electrostatic Potential Surface or (010) Kaolinite Clay



Passivant-Consolidation Coatings

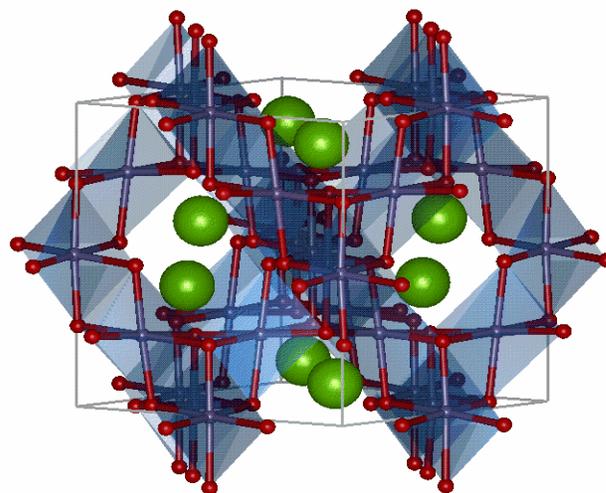
Energy minimizations of sol-gel coatings that best conform to carbonate surface and inhibit reaction

T = 300K
t = 15.6 psec



Metal Sorption on Clay Minerals

MD simulation of inner-sphere sorption of Cs⁺ ion onto aluminol site at (010) edge of kaolinite



Development of Battery Cathode Materials

Energy minimizations and MD studies of metal dopants on bulk structure and Li diffusion

Contact

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