Effect of Surface Parameters on Interfacial Water Film Behavior

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Effect of Surface Parameters on Interfacial Water Film Behavior
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Abstract
Vapor-to-liquid and liquid-to-solid transitions on mineral surfaces are the primary pathways for phase transitions in atmospheric water. These phase transitions affect the microphysics of clouds and have significant effects on the weather and climate. Our overall goal is to elucidate the mechanisms through which surfaces affect these transitions, and develop predictive abilities to correlate surface properties to the thermodynamics and kinetics of the phase transitions. In this work, we use molecular dynamics simulations to study the structure, and dynamics of water near kaolinite-like surfaces. Kaolinite is the most abundant mineral dust in the atmosphere. We specifically investigate the effect of lattice spacing on water structure in water films of varying thicknesses. Our results will help us ascertain the properties important to promote ice nucleation. The insights gained also have implications in designing materials that can prevent ice nucleation in applications such as power-lines, car windshields, and computer chips.

Overview of Molecular Dynamics Simulations
- Enables us to observe phenomena that occur over short time periods (nano-to-microseconds), and involve a small number of molecules (~100 to ~20,000 molecules). These length- and timescales are usually difficult to access in experiments.
- Allows us to decouple the effects of various parameters on the given system behavior.
- Provides a movie of the atoms in a system from which system properties can be calculated.

Surfaces: Kaolinite and modified kaolinite. The lattice spacing was increased and decreased by 10 and 20 % to generate modified kaolinite surfaces.
Monolayers: 1, 2 and 5ML. 1ML comprises 288 water molecules.
Temperature: 230, 250, 270 K
Total: 45 simulations, each for 1 μs

Future Work
- Use advanced sampling simulation techniques to generate the free energy landscape of liquid-to-solid transition for different surfaces.
- Calculate the rate of ice nucleation using forward flux sampling, an advanced technique to study rare events in simulations.

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