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Brittany Glatz
Clemson University

Luke Rhym
Clemson University

Sapna Sarupria
Clemson University

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Effect of Surface Parameters on Interfacial Water Film Behavior

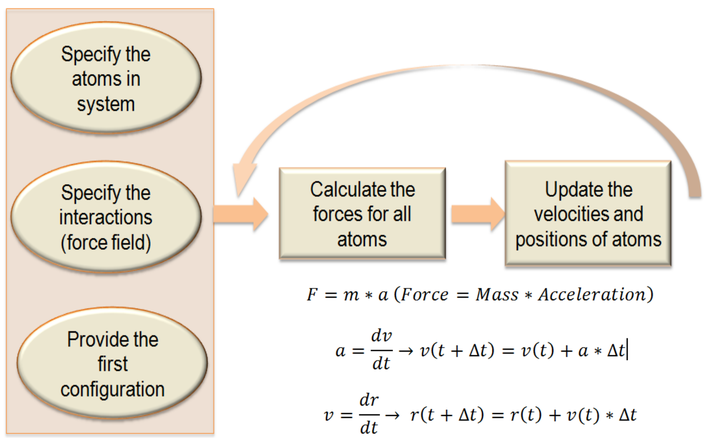
Brittany Glatz, Luke Rhym and Sapna Sarupria
Chemical and Biomolecular Engineering, Clemson University, Clemson SC 29634

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.

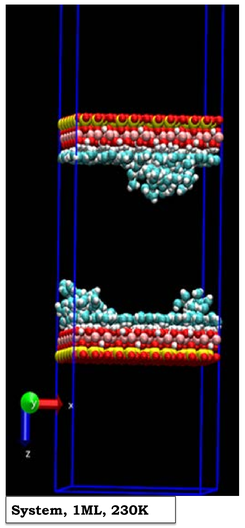
Overview of Molecular Dynamics Simulations

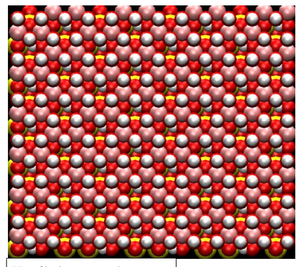
- Enables us to observe phenomena that occur over short time periods (nano-to-microseconds), and involve a small number of molecules (~100 to ~20,000 molecules). These length- and timescales are usually difficult to access in experiments.
- Allows us to decouple the effects of various parameters on the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

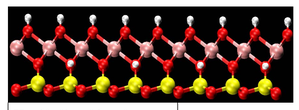


Acknowledgments: Palmetto Supercomputing at Clemson

Setup of Simulation System


System, 1ML, 230K


Kaolinite top view


Kaolinite side view

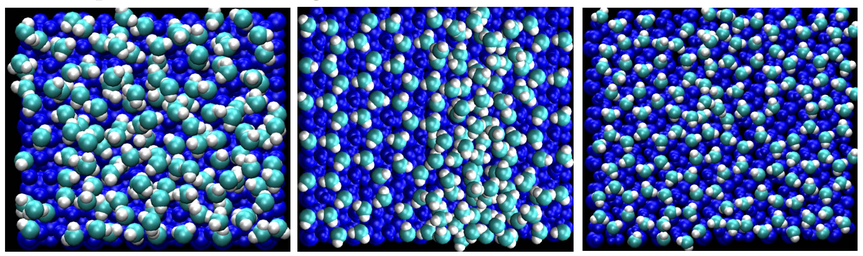
Kaolinite:
Red: Oxygen
White: Hydrogen
Pink: Aluminium
Yellow: Silicon
Water:
Cyan: Oxygen
White: Hydrogen

Force Fields:
Water: TIP4P/Ice
Kaolinite: CLAYFF
Software: GROMACS

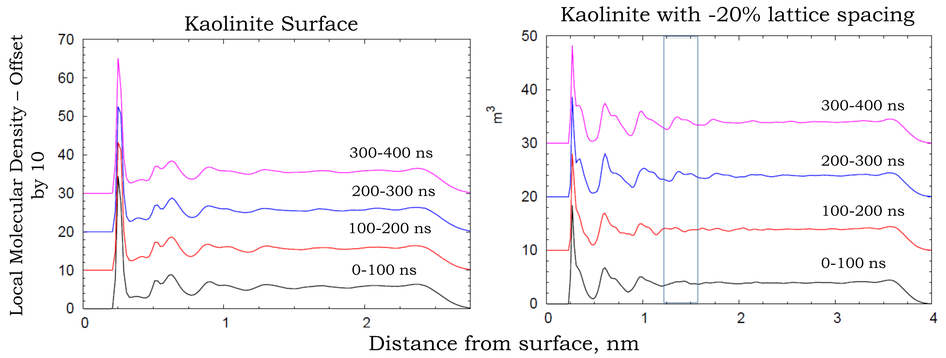
Surfaces: Kaolinite and modified kaolinite. The lattice spacing was increased and decreased by 10 and 20 % to generate modified kaolinite surfaces.
Monolayers: 1, 2 and 5ML. 1ML comprises 288 water molecules.
Temperature: 230, 250, 270 K
Total: 45 simulations, each for 1 µs

Computer time used for these simulations totals ~54 years!!

Top view of one configuration from the simulation, 1ML, 230K


Modified Kaolinite: -20% | Kaolinite | Modified Kaolinite: +20%

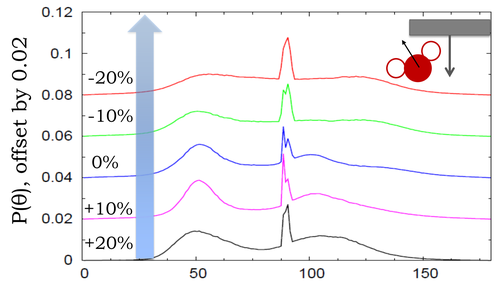
Water density for 5 ML at 230 K

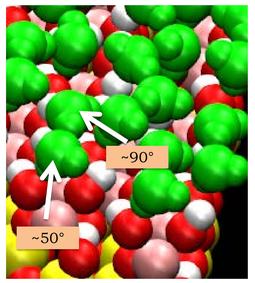


Decreased lattice spacing promotes ordering of water molecules for longer distances from the surface

Effect of Surface Lattice on Water Structure in 1ML Film at 230K

Angle Between Surface Normal and Water Dipole

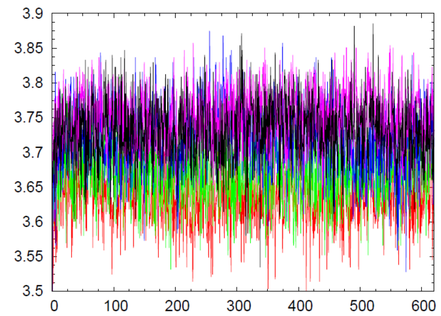


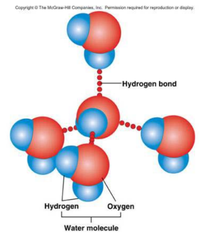


Water is shown in green

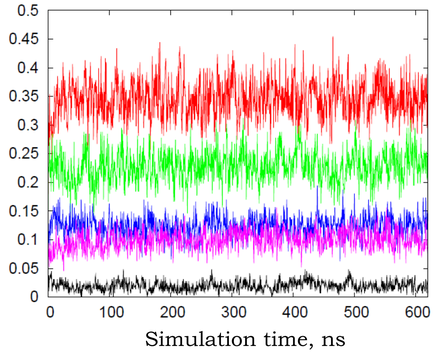
The flexibility of surface hydroxyl groups results water orienting with dipole angles around 50 and 90°

Number of Hydrogen Bonds per Water Molecule





Fraction of Solid Water Molecules



Water molecules are characterized as solid based on their tetrahedral arrangement as measured using the tetrahedral order parameter, q_i

$$q_i = \sum_{j=1}^{n_i-1} \sum_{k=j+1}^{n_i} \left(|\cos\theta_{jik}| \cos\theta_{jik} + \frac{1}{9} \right)^2$$

$q_i < 0.4$ for solid-like water molecules

Decreased lattice spacing results in increased tetrahedral order between water molecules to maintain the same number of hydrogen bonds per water molecule.

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.