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Water Structure and Its Correlation to Heterogeneous Ice Nucleation

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Water Structure and Its Correlation to Heterogeneous Ice Nucleation

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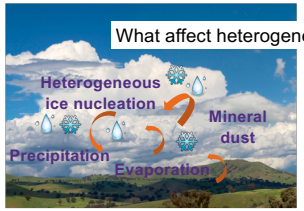
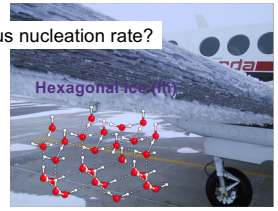
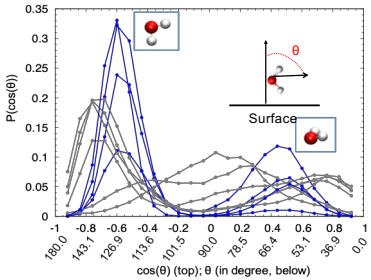
Heterogeneous Ice Nucleation

Water cycle

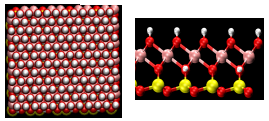


Ice on airplane





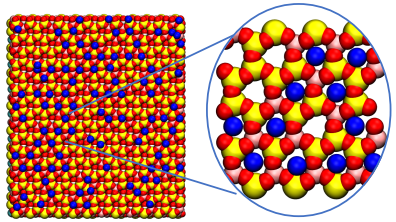
Kao surface[1]



Interfacial water structure in the metastable liquid state correlates with the propensity of observing ice nucleation at a given surface.

Probability distribution of dipole orientations of water: blue curves are surfaces that **promote** ice nucleation; grey curves are surfaces that **hinder** ice nucleation.

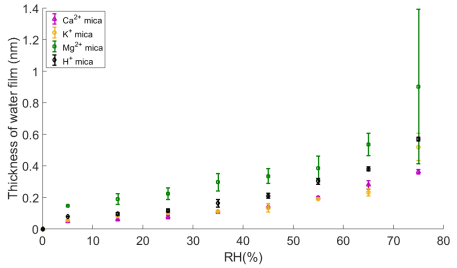
Mica Surface



Freshly cleaved muscovite mica contains K^+ ions. Washing mica with corresponding solutions can replace K^+ with other ions.

Red: oxygen, white: hydrogen, pink: aluminum, yellow: silicon, blue: sodium

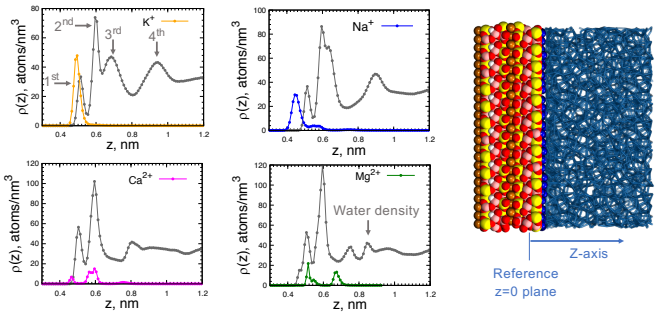
Water Adsorption Isotherms



Adsorption isotherms indicates the surface affinity of water. Each data point is composed of eight isotherms at different temperatures ranging from 5-23ºC. The increase of thickness of water is shown as a function of increasing RH.[2]

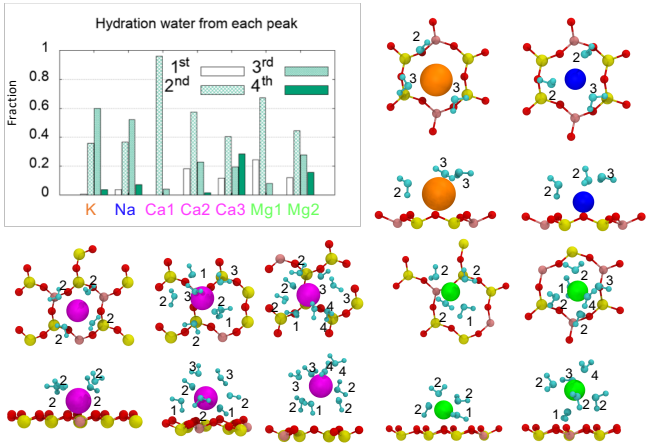
Mg^{2+}-mica has the highest water affinity among all the four mica surfaces.

Ion Adsorption and Hydration



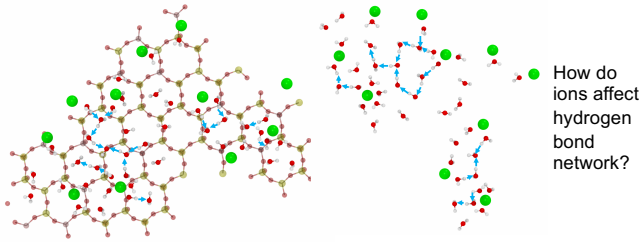
Ion density and water density on mica surfaces in z-direction at 300K. Grey curves are water density plots. A snapshot of simulation box is given on the right.

The interplay of ion-water, ion-surface, and surface-water interactions affect ion adsorption and water structure.



Ion hydration shell composition and snapshots. Labels on the snapshots indicate the water peak in density profile. Yellow, red, pink are mica surface atoms. Orange: K, blue: Na, magenta: Ca, green: Mg.

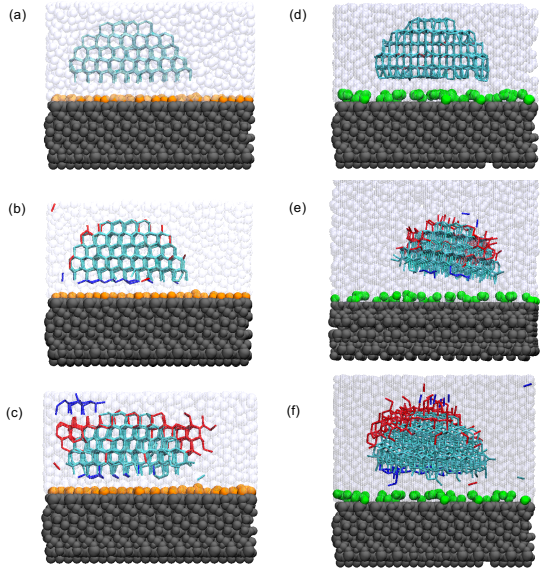
Monovalent ions mainly adsorb in the voids. Divalent ions have multiple adsorption states; both complete hydration and partial hydration is observed.



How do ions affect hydrogen bond network?

Hydrogen bond network in Mg^{2+}-mica. Blue arrows indicate hydrogen bond between water molecules.

Ice Nucleation via Seeding



Hexagonal basal plane seed with a radius of 2 nm on K^+-mica (a, b, and c) and Mg^{2+}-mica (d, e, and f) at 235 K. Gray: mica surface, cyan: original seed, blue: cubic ice, red: hexganoal ice, ice blue: liquid water, orange: K, green: Mg. panel (a) and (d): seed at the beginning of equilibration; panel (b) and (e): growth of ice around seed at the end of equilibration run; panel (c) and (f): growth of ice around seed at the end of 50 ns production run.

Seeds grow differently on K^+-mica and Mg^{2+}-mica.

Tilting has been observed to affect the further growth near the seed.

The ability of ion to localize water molecules influences seed growth.

Conclusions and Future Work

- Ion hydration influences water structure. Mg^{2+} ions have the strongest ability to restructure water in vicinity.
- Further investigation on mechanism of ice nucleation via seeding and water dynamics, along with freezing experiments on different mica systems helps elucidating the role of surfaces in heterogeneous ice nucleation.

References

1. Brittany Glatz, Sapna Sarupria, *Langmuir* 2018 *34* (3), 1190-1198
2. Will Cantrell, George E. Ewing, J. Phys. Chem. B 2001, 105, 5434-5439
3. **Jiarun Zhou**, Nurun N. Lata, Sapna Sarupria, Will Cantrell, to be submitted

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