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Towards the surface science of ice nucleation on aqueous organic solutions and solid substrates

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The nucleation of ice is an important process in chemistry, physics and atmospheric science. Although ice nucleation has been studied since long, our understanding of ice nucleation is still far from complete, particularly from a molecular point of view. The hydrogen bonding structure of H_2O can be significantly different between liquid water to ice. This structure is responsible for most of the difference in physical and chemical properties between the different aggregation states of water. The difference between the hydrogen bonding structure of liquid water and ice can be experimentally observed by near edge X-ray absorption fine structure (NEXAFS) spectroscopy at the oxygen K-edge, because it involves resonant transitions into unoccupied molecular orbitals, which are very sensitive to the nearest neighbors of oxygen atoms. NEXAFS spectroscopy can be performed in electron yield mode, in which Auger electrons emitted upon initial core hole excitation are detected, which provides a surface sensitive NEXAFS spectrum. Experiments reported in this work were performed at the near ambient photoelectron spectroscopy endstation (NAPP) at the SIM and NANOXAS beamline at the Swiss Light Source (PSI, SLS).

Since it has been suggested that some organic compounds have the potential to modify the structure of water that influences the nucleation of ice, we have measured electron yield NEXAFS spectra from a liquid jet of aqueous solution containing tetrabutylammonium bromide (TBAB). The O K-edge spectra exhibit a clear change in the relative features. These features represent hydrogen bonding at different level, indicating that the cationic head group of TBAB induces a significant variation of the hydrogen bonding network near the surface of the aqueous solution.

On the other hand, the hydrogen bonding structure of adsorbed water on a solid substrate may control deposition nucleation, which is another pathway of heterogeneous ice nucleation. The hydrogen bonding structure may be affected by short and long range interactions between the substrate and the adsorbed water molecules. As a first approach, we have measured electron yield NEXAFS spectra of adsorbed water on graphite and titanium dioxide (TiO_2) under subsaturated conditions with respect to ice. Under isobaric conditions and by varying the temperature of the sample, we can change the relative humidity, which leads to varying amounts of adsorbed water in equilibrium between the substrate and water vapor. Preliminary results show that, under different relative humidity, the weakly and strongly coordinated OH bond of adsorbed water on TiO_2 and graphite show different contributions to the Auger electron yield NEXAFS spectrum, that is, the resonant transitions near the oxygen K-edge vary with relative humidity and temperature. We attribute this to the modification of the organization of water molecules in response to the interactions with the solid substrate. In view of the application of the NEXAFS technique, we believe it opens up a powerful tool to address the surface science of ice nucleation in the future.