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Fundamentals of acid-base chemistry at and in the quasi-liquid-layer

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Earth's surface snow plays an active part in atmospheric chemistry. Research over the past decades has provided an impressive observational basis of the resulting large scale effects, such as substantial modification of the composition and of the chemical reactivity of the lowermost atmosphere in polar regions.

Here, I present details on the chemical mechanisms operating in environmental snow and ice derived from well controlled laboratory based experiments. The research is taking full advantage of the Near Ambient Pressure Photoelectron spectroscopy (NAPP) end station at PSI/SLS reveals the ability of atmospheric trace gases to modify the structure of ice at the upper few nanometers at the air-ice interface upon adsorption. Using near ambient pressure core level X-ray photoelectron spectroscopy, we directly detected depth profiles and dissociation degree of adsorbed acidic trace gases at 230 - 255 K at low surface coverage. Complementary X-ray absorption measurements (NEXAFS) show how the presence of acid induces changes to the hydrogen bonding network in the interfacial region.

We interpret the data as
* a Janus-type character of physisorbed molecular acid at the outermost ice surface and dissociation occurring upon solvation deeper in the interfacial region.
* a non-uniform of chemical and physical properties of the hydrogen bonding network along the depth of the QLL

Even with a focus of this presentation on adsorption of acidic trace gases (HCl, HNO3, formic acid, acetic acid) to ice and on the molecular structure of the hydrogen bonding network at the air-ice interface, the details on chemistry at extreme concentration and temperature conditions at interfaces might be of high relevance not only in environmental science but also in general chemistry, material science, catalysis, cryobiology, and astrophysics.

Significance statement

These data describe the chemical properties of the air-ice interface and question the general applicability of the acid-base concept across interfaces.

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