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Surface-specific spectroscopy of water and ice

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Water and ice surfaces and interfaces are ubiquitous, not just in nature (e.g. for various naturally occurring forms of snow and ice) but also in many technological applications (such as food science and artificial snow machines). Water is a rather unique liquid, owing to its strong intermolecular interactions: strong hydrogen bonds hold water molecules together. At the surface of ice, the water hydrogen-bonded network is abruptly interrupted, conferring distinct properties on the interface compared to bulk.
We elucidate the structure of interfacial water molecules at the surface of solid ice, and of water in contact with different materials, using surface-specific vibrational spectroscopy of interfacial water molecules. For ice, we find an excess of hydrogen bonds at the ice-vapor interface around 200 K, due to a competition between entropic and enthalpic contributions to the free energy. Around 250 K temperatures, surface melting of ice is found to occur in a bilayer-by-bilayer fashion. Finally, we relate the temperature-dependent molecular structure of the ice surface to the macroscopic friction coefficient, and explain why ice is most slippery around 264 K.

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