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Surface Studies of Ice[1]

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Despite ice being a ubiquitous and well-studied substance, it is surprising that some basic questions about its surface properties are still debated. Here computer simulations are used to study the unusual structure and dynamics of ice surface at atomic scale. An order parameter, which defines the ice surface energy, is identified for the first time. A classical electrostatic model proves useful to explain the physics inside. We predict that the proton order-disorder transition, which occurs in the bulk at ~ 72 K, will not occur at the surface at any temperature below surface melting. In addition, we find that the surface of crystalline ice exhibits a remarkable variance in vacancy formation energies that is more characteristic of an amorphous material. A fraction of surface molecules are bound by less than the strength of a single hydrogen bond, yet other sites are more strongly bound than those in the crystal interior. Vacancy energies are found to be as low as ~ 0.1eV at the surface, leading to a higher than expected concentration of vacancies at the external layer. Once a surface vacancy is formed, the energetic cost of forming neighbouring vacancies is greatly reduced, facilitating pits on the surface and other processes that may contribute to the phenomenon of pre-melting and quasi-liquid layer formation. Finally, we show that the distribution of local arrangement of dangling atoms, characterized by a surface proton order parameter, is also of crucial importance for the adsorption of water monomer on ice surface. The positive correlation of adsorption energy of water monomer with surface proton ordering suggests that the adsorption may prefer to firstly occur in the inhomogeneous surface, which sheds light on our understanding of the ice nucleation and growth as well as other physical/chemical reactivity in high altitude clouds.

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