Abstract template:

Title

Proton order in the ice crystal surface

Reference

PNAS **2008**, *105*, 5969-5974

Authors

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Abstract

The physics of the ice crystal surface and its interaction with adsorbates are not only of fundamental interest but also of considerable importance to terrestrial and planetary chemistry. Yet the atomic-level structure of even the pristine ice surface at low temperature is still far from well understood. This computational study focuses on the pattern of dangling H and dangling O (lone pairs) atoms at the basal ice surface. Dangling atoms serve as binding sites for adsorbates capable of hydrogen- and electrostatic bonding. Extension of the well known orientational disorder (‘‘proton disorder’’) of bulk crystal ice to the surface would naturally suggest a disordered dangling atom pattern; however, extensive computer simulations employing two different empirical potentials indicate significant free energy preference for a striped phase with alternating rows of dangling H and dangling O atoms, as suggested long ago by Fletcher [Fletcher NH (1992) *Philos Mag* 66:109–115]. The presence of striped phase domains within the basal surface is consistent with the hitherto unexplained minor fractional peaks in the helium diffraction pattern observed 10 years ago. Compared with the disordered model, the striped model yields improved agreement between computations and experimental *ppp*-polarized sum frequency generation spectra.