Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Role of proton ordering in adsorption preference of polar molecule on ice surface ZHAORU SUN, Peking University, Beijing, P.R. China, DING PAN, University of California, Davis, CA, LIMEI XU, ENGE WANG, Peking University, Beijing, P.R. China — Adsorption of polar monomers on ice surface, relevant to the physical/chemical reaction in ice clouds as well as growth of ice, remains an open issue partially due to the unusual surface characteristics with protons at the top layer of ice. Using first-principle calculations, we explore the adsorption properties of ice surface in terms of a surface proton order parameter, which characterizes the inhomogeneity of the dangling atoms on ice surface. We show that, due to an effective electric field created by dangling OH bonds and lone pairs of water molecules not only directly neighboring but also further away from the adsorbed polar molecule on the ice surface, the adsorption energy of polar monomer on ice surface exhibits large variance and a strong correlation with the proton order parameter of ice surface. Our results about the positive correlation between the inhomogeneity of ice surface and adsorption energies suggest that the physical/chemical reactions as well as the growth of ice may prefer to occur firstly on surfaces with larger proton order parameter.

Zhaoru Sun
Peking University, Beijing, P.R. China

Date submitted: 10 Dec 2012 Electronic form version 1.4