

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**First-principles study of the infrared spectrum of the ice Ih (0001) surface**<sup>1</sup> HUANG PATRICK, Lawrence Livermore National Laboratory, Livermore, California, 94550, T. ANH PHAM, University of California, Davis and Lawrence Livermore National Laboratory, Livermore, California, 94550, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, Livermore, California, 94550, GIULIA GALLI, University of California, Davis — Ice particles catalyze a number of processes relevant to atmospheric and environmental chemistry, and the elucidation of these reactions require knowledge of the ice surface structure. Although it is well known that the structure of bulk ice-Ih is proton disordered, the understanding of the microscopic structure of the ice surface is still limited. Recent theoretical studies <sup>1,2</sup> suggest that the basal (0001) surface of ice Ih is significantly more proton ordered than the bulk. In this work we compute infrared (IR) spectra of several ordered and disordered models of the (0001) surface of ice, and investigate the sensitivity of these spectra to the microscopic details of the surface structure. In particular we discuss possible signatures of disorder in the computed spectra. [1] D. Pan et al., Phys. Rev. Lett. 101, 155703 (2008); [2] V. Buch et al., Proc. Natl. Acad. Sci. U.S.A. 105, 5969 (2008)

<sup>1</sup>Prepared by LLNL under Contract DE-AC52-07NA27344

T. Anh Pham  
University of California, Davis and Lawrence Livermore  
National Laboratory, Livermore, California, 94550

Date submitted: 28 Nov 2011

Electronic form version 1.4