Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Ab initio structure and energetics of ice Ih - implications for wetting[1] PETER J. FEIBELMAN, Sandia National Laboratories — The lattice energy of ice Ih is found to equal 0.68 eV/H_2O, in a VASP-based, GGA/PW91 optimization of a 96-molecule cell, with zero dipole moment in every hexagonal layer.[2] This result agrees closely with Hamann's value, obtained for a small, proton-ordered, and thus polarized unit cell.[3] Slight inhomogeneous broadening of the O-H stretch peak is estimated, based on the computed O-O distance distribution. Implications regarding wetting-layer formation will be discussed.

[1]Supported by the DOE Office of Basic Energy Sciences. Sandia is operated by the Lockheed Martin Co. for USDOEs National Nuclear Security Administration under Contract DE-AC04-94AL85000.
[2]J. A. Hayward, J. R. Reimers, J. Chem. Phys. **106**, 1518(1997).
[3]D. R. Hamann, private communication. See, P. J. Feibelman, Science **295**, 99(2002), ref. 19.

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Date submitted: 21 Nov 2005 Electronic form version 1.4