Ab initio structure and energetics of ice Ih - implications for wetting

PETER J. FEIBELMAN, Sandia National Laboratories — The lattice energy of ice Ih is found to equal 0.68 eV/H$_2$O, in a VASP-based, GGA/PW91 optimization of a 96-molecule cell, with zero dipole moment in every hexagonal layer. This result agrees closely with Hamann’s value, obtained for a small, proton-ordered, and thus polarized unit cell. 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.

1Supported 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.
