

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Effects of Thermal and Quantum Fluctuations on Dipole-moment distribution of H_2O molecules in ice I_h ¹ PEDRO MOREIRA, UFSCar, MAURICE DE KONING, Unicamp — Molecular dipole moments are the fundamental entities that underpin the dielectric behavior of molecular materials. Here, we discuss the molecular-dipole distributions of water molecules in ice I_h , considering the roles of proton-disorder, as well as the effects of thermal and quantum fluctuations. For this purpose we employ *ab initio* Born-Oppenheimer and Path-Integral Molecular Dynamics simulations and compute molecular dipole moments using maximally-localized Wannier functions. We discuss trends in the dipole-moment distributions as a function of temperature.

¹P.A.F.P.M. and M.K. acknowledge financial support from the Brazilian agencies Fapesp, Capes, and CNPq. All calculations were performed at CCJDR, IFGW, Unicamp.

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Date submitted: 14 Nov 2014

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