Effects of Thermal and Quantum Fluctuations on Dipole-moment distribution of $H_2O$ molecules in ice $I_h$\textsuperscript{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 \textit{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.

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