Title: Hydrogen bond symmetrization in high pressure ice

Author: Marco Cherubini

Abstract:
The symmetrization of the hydrogen bond length in high pressure ice, associated with the phase transition from ices VII-VIII to ice X, is a long-time debated issue because of the lack of clear and unambiguous experimental signatures. Here, we simulate the structural and thermodynamic properties of the phase transition by employing the stochastic self-consistent harmonic approximation to include quantum anharmonicity at a non-perturbative level. We prove the strength of quantum fluctuations in this system showing that the inclusion of quantum effects induces a 65 GPa reduction of the classical critical pressure at 0K (from 116 GPa to around 50 GPa) and makes it completely temperature independent in a wide range (50-300K), in opposition with the strongly nonlinear temperature dependence regime we observe in the classical approximation.
Furthermore, we show that proton order affects negligibly the hydrogen bond symmetrization. Within the SSCHA framework, we observe that the phase transition between VII-X and VIII-X occurs, within 4 GPa, at the same pressure, around 50 GPa, that is in a good agreement with the indirect experimental estimation obtained through spectroscopy. Finally, we manage to reproduce perfectly the 10 GPa isotope shift due to the hydrogen-to-deuterium substitution.