Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Nuclear quantum effects in high-pressure ice YAEL BRONSTEIN, PHILIPPE DEPONDT, FABIO FINOCCHI, Universite Pierre et Marie Curie —
Because of their mass, hydrogen nuclei are subjected to nuclear quantum effects (NQE), mainly tunneling and zero-point energy. They can be crucial to describe correctly the properties of H-containing systems, even at room temperature. A prototypical example of the importance of NQE is the transition from asymmetric H-bonds in phase VII to symmetric bonds in phase X of high-pressure ice, in which NQE drastically reduce the transition pressure [1]. However, natural ice is rarely pure and even small concentrations of salt (LiCl or NaCl) in ice have a strong effect on the phase diagram: the VII to X transition is shifted to higher pressures, questioning the resilience of NQE in the presence of ionic impurities [2]. We investigate these questions using the Quantum Thermal Bath [3], a semi-classical Langevin dynamics, taking into account both NQE and thermal effects in pure and salty ices. We show why NQE can be sensitive to the presence of impurities and that non-trivial phenomena could result, such as the spectacular upshift of the transition pressure and the peculiar motion of ions.

[1]Benoit et al, Nature 392, 258 (1999); Bronstein et al, Phys. Rev. B 89, 214101 (2014)
[2]Bove et al, PNAS 112, 8216 (2015)
[3]Dammak et al, Phys. Rev. Lett. 103, 190601 (2009)

Yael Bronstein
Universite Pierre et Marie Curie

Date submitted: 05 Nov 2015 Electronic form version 1.4