Abstract Submitted
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Anatomy of competing quantum effects in liquid water. RAFA RAMIREZ, Instituto de Ciencia de Materiales de Madrid (ICMM), SRIRAM GANESHAN, University of Maryland, College Park, M. V. FERNANDEZ-SERRA, Stony Brook University — ct- Molecules like water have vibrational modes with zero point energy well above room temperature. As a consequence, classical molecular dynamics simulations of liquid water largely underestimate the kinetic energy of the ions, which translates into an underestimation of covalent interatomic distances. In this work, we show that it is possible to apply generalized Langevin equation with suppressed noise in combination with Nose-Hoover thermostats to achieve an efficient zero-point temperature of independent modes of liquid water. Using this method we deconstruct the competing quantum effects in liquid water. We demonstrate how the structure and dynamical modes of liquid water respond to non-equilibrium distribution of zero point temperatures on the normal modes.

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