Abstract Submitted
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Nuclear quantum effects in water[1] JOSEPH MORRONE, ROBERTO CAR, Dept. of Chemistry, Princeton University — In this work, a path integral Car-Parrinello molecular dynamics[2] simulation of liquid water is performed. It is found that the inclusion of nuclear quantum effects systematically improves the agreement of first-principles simulations of liquid water with experiment. In addition, the proton momentum distribution is computed utilizing a recently developed "open" path integral molecular dynamics methodology[3]. It is shown that these results, which are consistent with our computations of the liquid structure, are in good agreement with neutron Compton scattering data[4]. The remaining discrepancies between experiment and the present results are indicative of some degree of over-binding in the hydrogen bond network, likely engendered by the use of semi-local approximations to density functional theory in order to describe the electronic structure.

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[2]CPMD V3.11 Copyright IBM Corp 1990-2006, Copyright MPI fuer Festkoerperforschung Stuttgart 1997-2001.
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