

Abstract Submitted  
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**Large-Scale Hybrid Density Functional Theory Calculations in the Condensed-Phase: *Ab Initio* Molecular Dynamics in the Isobaric-Isothermal Ensemble**<sup>1</sup> HSIN-YU KO, BISWAJIT SANTRA, Princeton University, ROBERT A. DISTASIO JR, Cornell University, XIFAN WU, Temple University, ROBERTO CAR, Princeton University — Hybrid functionals are known to alleviate the self-interaction error in density functional theory (DFT) and provide a more accurate description of the electronic structure of molecules and materials. However, hybrid DFT in the condensed-phase has a prohibitively high associated computational cost which limits their applicability to large systems of interest. In this work, we present a general-purpose order(N) implementation of hybrid DFT in the condensed-phase using Maximally localized Wannier function; this implementation is optimized for massively parallel computing architectures. This algorithm is used to perform large-scale *ab initio* molecular dynamics simulations of liquid water, ice, and aqueous ionic solutions. We have performed simulations in the isothermal-isobaric ensemble to quantify the effects of exact exchange on the equilibrium density properties of water at different thermodynamic conditions. We find that the anomalous density difference between ice *Ih* and liquid water at ambient conditions as well as the enthalpy differences between ice *Ih*, II, and III phases at the experimental triple point (238 K and 20 Kbar) are significantly improved using hybrid DFT over previous estimates using the lower rungs of DFT. [1] X Wu, A Selloni, and R Car, PRB 79, 08510

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