Abstract Submitted
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Local Structure in *Ab Initio* Liquid Water: Signatures of Amorphous Phases[1] BISWAJIT SANTRA, Princeton University, Princeton, USA, ROBERT A. DISTASIO, JR., Cornell University, Ithaca, USA, FAUSTO MARTELLI, ROBERTO CAR, Princeton University, Princeton, USA — Within the framework of density functional theory, the inclusion of exact exchange and non-local van der Waals/dispersion interactions is crucial for predicting a microscopic structure of ambient liquid water that quantitatively agrees with experiment [1]. In this work, we have used the local structure index (LSI) order parameter to analyze the local structure in such highly accurate *ab initio* liquid water. At ambient conditions, the LSI probability distribution, P(I), was unimodal with most water molecules characterized by more disordered high-density-like local environments. With thermal excitations removed, the resultant bimodal P(I) in the inherent potential energy surface (IPES) exhibited a 3:1 ratio between high- and low-density-like molecules, with the latter forming small connected clusters amid the predominant population. By considering the spatial correlations and hydrogen bond network topologies *among* water molecules with the same LSI identities, we demonstrate that the signatures of the experimentally observed low- and high-density amorphous phases of ice are present in the IPES of ambient liquid water [2]. [1] DiStasio *et al.*, J. Chem. Phys. **141**, 084502 (2014). [2] Santra *et al.*, Mol. Phys. **113**, 2829 (2015).

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