Abstract Submitted
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A Dataset of First-Principles Molecular Dynamics Simulations of Water[1] FRANCOIS GYGI, WILLIAM DAWSON, Univ of California - Davis — We present a dataset of first-principles molecular dynamics simulations [1] of water performed using Density Functional Theory. A set of 32 independent 64-molecule samples was used in separate, parallel simulations for a duration of 58 ps. An analysis of atomic trajectories is given focusing on correlations of the Kohn-Sham energy, ionic kinetic energy, pair correlation functions, diffusion coefficient, and vibrational spectrum. The availability of 32 independent simulations allows for an estimation of the variance of averaged quantities, both within MD runs and between samples. The variability of oxygen pair correlation functions across samples provides a measure of the uncertainty associated with that quantity. We observe several instances of large fluctuations in the oxygen pair correlation functions that can be associated with increases in the local structure index (LSI) proposed by Shiratani and Sasai [2] supporting the hypothesis that water undergoes frequent changes to locally highly structured configurations. Complete atomic trajectories and simulation output files are available online[3].
[1] Qbox code, http://eslab.ucdavis.edu/software/qbox
[2] E. Shiratani and M. Sasai, J. Chem. Phys. **104**, 7671 (1996)
[3] http://www.quantum-simulation.org

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