Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Study of correlations from Ab-Initio Simulations of Liquid Water[1]

ADRIAN SOTO, MARIVI FERNANDEZ-SERRA, Stony Brook University, DEYU LU, SHINJAE YOO, Brookhaven National Laboratory — An accurate understanding of the dynamics and the structure of H2O molecules in the liquid phase is of extreme importance both from a fundamental and from a practical standpoint. Despite the successes of Molecular Dynamics (MD) with Density Functional Theory (DFT), liquid water remains an extremely difficult material to simulate accurately and efficiently because of fine balance between the covalent O-H bond, the hydrogen bond and the attractive the van der Waals forces. Small errors in those produce dramatic changes in the macroscopic properties of the liquid or in its structural properties. Different density functionals produce answers that differ by as much as 35% in ambient conditions, with none producing quantitative results in agreement with experiment at different mass densities [J. Chem Phys. 139, 194502(2013)]. In order to understand these differences we perform an exhaustive scanning of the geometrical coordinates of MD simulations and study their statistical correlations with the simulation output quantities using advanced correlation analyses and machine learning techniques.

---

[1] This work was partially supported by DOE Award No. DE-FG02-09ER16052, by DOE Early Career Award No. DE-SC0003871, by BNL LDRD 16-039 project and BNL Contract No. DE-SC0012704.

Adrian Soto
Stony Brook University

Date submitted: 24 Nov 2015

Electronic form version 1.4