

Abstract Submitted
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Correcting for the Self-Interaction Error in Ab-Initio Molecular Dynamics Simulations ALESSANDRO GENOVA, Rutgers University - Newark , DAVIDE CERESOLI, CNR, ISTM, ALISA KRISHTAL, MICHELE PAVANELLO, Rutgers University - Newark — The Self-Interaction Error (SIE) in semilocal Kohn-Sham (KS) DFT is omnipresent and it can strongly affect the quality of the properties predicted by ab-initio molecular dynamics (AIMD). Liquid water offers two good examples of this behavior: (1) semilocal KS-DFT overestimates the hydrogen bond strength resulting in an overly structured liquid, similar to ice; (2) in the case of solvated radical species, such as OH, KS-DFT exhibits unphysical spin density leakage to neighboring water molecules. We identify the cause of such behavior to be the SIE in the interaction between different molecules (rather than within). Unfortunately, it is a challenge to only rid of the SIE in the intermolecular interactions without introducing spurious corrections for the intramolecular interactions. Semilocal formulations of subsystem DFT offer an elegant solution to this problem: they remove the intermolecular self interaction, and result in an optimal description of liquid water and solvated OH radical, as compared against the experiment. In addition, the subsystem DFT simulations involve a much reduced computational effort compared to KS-DFT. [1] A. Genova et al., JCP 2014, 141, 174101 [2] A. Genova et al., JPCM 2015, Accepted

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