

Abstract Submitted
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Failure of popular density functionals: Torsional potential of conjugated hetero double bonds DIANA TAHCHIEVA, ANATOLE VON LILIENFELD, University of Basel — Accurate predictions of torsional potential energy profiles are crucial to correctly sample conformational degrees of freedom. Using most of currently popular density functionals we have investigated many small organic closed shell molecules with conjugated hetero double bonds. Typically, density functional theory (DFT) is assumed to provide reasonable energy estimates for such systems and properties. In comparison to CCSD(T), however, all functionals fail to quantitatively reproduce the correct potential, except for M0(5,6)2X and CAM-B3LYP. For molecules containing CO or CS double bonds and heavy halogene atoms even qualitative trends can not be recovered. Analysis of the results reveals that the deviations are due to large errors in the electrostatic potential originating in a failures to generate correct electron densities. Empirical atom centered corrections can rectify some of the short-comings for PBE and BLYP [1].

[1] D. Tahchieva, R. Ramakrishnan, O. A. von Lilienfeld, in preparation (2016)

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