

PERFORMANCE OF SCAN DENSITY FUNCTIONAL FOR A SET OF IONIC LIQUID ION PAIRS

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Ionic liquids (IL) have been extensively studied due to their high thermal and electrochemical stability, which makes them suitable candidates for energy storage applications, catalysis, and many other applications [1]. Computational chemistry is a powerful tool for searching materials with the desired properties, including ionic liquids for electrochemical applications. Herein, the choice of the computational method is not trivial, as it has to be both efficient and accurate. Density functional theory methods with appropriate corrections can give precision close to that of the post-Hartree–Fock coupled cluster methods with a fraction of their cost [2].

Thence, we have evaluated the performance of a recently developed non-empirical strongly constrained and appropriately normed (SCAN) [3] density functional on electronic structure calculations of ionic liquid ion pairs. The performance of SCAN and other popular functionals (PBE, M06-L, B2PLYP) along with Grimme's dispersion correction and Boys–Bernardi basis set superposition error correction was compared to DLPNO-CCSD(T)/CBS. We show that SCAN reproduces coupled-cluster results for describing the employed dataset of 48 ion pairs [4].

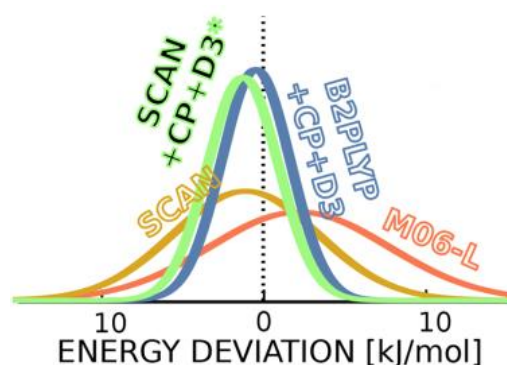


Fig.1 Deviation distribution of ion pair interaction energies compared to the reference method.

References

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