Performance of DFT methodologies using momentum space quantum similarity on diatomic molecules

Jelle Vandenbussche, Guillaume Acke, Patrick Bultinck

Department of Inorganic and Physical Chemistry, Ghent University, Krijgslaan 281 (S3), jelle.vandenbussche@UGent.be

Momentum space quantum similarity measures or mQSM$^{1-5}$ have proven to be useful because of the emphasis on the outer valence of the electron density which is of utmost interest to chemists. In the present study on 24 diatomic molecules we address the performance of several quantum chemical techniques by comparing the calculated mQSM with results obtained for CISD. These techniques include HF, MP2 and a total of 10 DFT methods. Unlike previous studies$^6$, our study includes recently developed DFT methodologies and shows that some DFT functionals perform better than HF. MP2 is however better than any of the DFT methods. The best performing functionals are B3PW91, MPW1PW91 and PBE1PBE.

References: