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Comparative Study of the Performance of DFT B3PW91 for the Prediction of Electronic Properties of Molecules JASMA BATHAM, PEDRO DEROSA, Louisiana Tech University — Density Functional Theory is a widely used and accepted tool for the prediction of ground state molecular properties. However and despite the fact that the hybrid GGA functional B3PW91 has proven to be successful for many application, its use seems not to be as widespread. In a paper by Zhang and Musgrave the HOMO, the LUMO and the energy difference between the two (HLG), is compared for a set of 27 molecules to the experimental ionization potential (IA), electron affinity (EA), and the lowest excitation energy respectively. The first two are inspired by the Koopman's theorem that suggests that the HOMO is a good approximation of -IP while the negative of the LUMO is an approximation of the -EA. Notably, in the mentioned paper, results for 11 different DFT functional are compared but B3PW91 is not one of them. In this work we compare the performance of B3PW91, to that of B3LYP, also a hybrid functional, and the corresponding non-hybrid GGAs BLYP and BPW91 for the same 27 molecules. For all the cases the 6-311+G** basis set is used. We compare HOMO, LUMO and HLG to the experimental IP, EA, and first excitation energy among the four methods. In addition we formally calculated the IP and EA as the difference in energy between the corresponding ion and the neutral. B3PW91 show at least comparable results to other methods more commonly used.

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