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POS-32 Assessment of the Performance of Four Dispersion-Corrected DFT Methods Using Optoelectonic Properties and Binding Energies of Organic Monomer-Fullerene Pairs

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With the aid of different polymer materials, intermolecular interactions, energy levels, and optical absorption spectra of polymers and fullerenes can be adjusted so as to enhance the efficiencies of heterogeneous organic solar cells. It is known that computational simulations such as density functional theory (DFT) can play an important role in identifying polymers with favourable properties and hence in speeding up the process of designing organic solar cells with higher efficiencies. However, what is often not known is which one of the dispersion-corrected DFT (D-DFT) methods gives the most accurate results (relative to the experimental data) for the various properties of conjugated systems such as are found in heterogeneous organic solar cells. In this study, we employ four D-DFT methods (such as ωB97x-D, B97-D3, B3LYP-D3, and PBE1PBE-D3) to calculate the binding energies and, using the D-DFT optimized geometries, we perform single point DFT/B3LYP calculations to obtain HOMO and LUMO eigenvalues, and HOMO-LUMO band gaps of the various (promising) molecular pairings of organic monomers and fullerenes. In addition, we employ time dependent DFT (TD-DFT) to obtain the maximum absorption wavelengths of the monomers of interest. Our results show that B97-D3 and B3LYP-D3 computations give the largest binding energies relative to the other D-DFT methods and they yield (relative to experimental values) the most accurate electronic and absorption results. This study provides a detailed comparison of results as obtained using the four D-DFT methods for the various properties of the monomer/fullerene combinations.

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