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Theoretical and Computational Investigation of PCBM and PC71BM Derivatives using the DFT Method

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Abstract : Organic photovoltaic cells are electronic devices that convert sunlight into electricity. To this end, the number of studies on organic photovoltaic cells (OVCs) is growing, and this trend is expected to continue. Computational studies are still needed to verify and prove the capability of CVOs, specifically the nanometer molecule PCBM, based on successful experimental results. In this paper, we present a theoretical and computational investigation of PCBM and PC71BM derivatives using the DFT method. On this basis, we employ independent and time-dependent density theories. HOMO, LUMO and GAPH-L energies, ionization potentials and electronic affinity are determined and found to be in agreement with experiments. Using DFT theory based on B3LYP and M062X methods with bases 6-31G (d,p) and 6-311G (d), calculations show that the most efficient acceptors are presented in the group of PC71BM derivatives and are in substantial agreement with experiments. The geometries of the structures are optimized by Gaussian 09.

Keywords : PCBM, P3HT, organic cell solar, DFT, TD-DFT
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