Energy level gamut, a wide-angle lens to look at photoelectronic properties of Diketopyrrolopyrrole-~~Benzothiadiazole~~ Benzothiadiazole-based small molecules

https://link.springer.com/article/10.1007/s00894-019-4110-8#citeas

Abstract: Demands in the molecular design for an optimized bandgap and proper energy levels to obtain high efficiencies are progressively growing ~~in the case of~~regarding organic electronics. In the present work, we design a series of molecules based on diketopyrrolopyrrole (DPP) and benzothiadiazoles (BT). We also study the presence and position of the nitrogen atom as an effective heteroatom. Finally, we optimize energy levels of the designed structures to ~~figure out~~discover the most favorable donor properties along with fullerene and non-fullerene (NF) acceptors in BHJ solar cell systems.

We develop a correction gamut of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels for the designed molecules. The gamut is a span with the ~~highest~~ maximum probability of occurrence of HOMO and LUMO of the designed molecule in the solution or solid state when they are derived from DFT computations in the gas phase. The model was validated by experimental energy level values of a similar structure as a reference material.

The ~~obtained~~ results obtained by the new ~~pathway~~ solution of combining the idea of energy level gamuts and ~~improved~~ improving Scharber model for NF BHJ ~~show~~ suggested that the designed structures can afford 8.5 to 10.5 % power conversion efficiencies (PCE) for NF-BHJ.