# New donor materials for bulk-heterojunction solar cells

**DFT and TD-DFT studies of new pentacene-based organic molecules as a donor material for bulk-heterojunction solar cells**

The performance of organic cells based on bulk heterojunctions (BHJs) has improved recently, but further improvements are necessary. In this work, we have carried out a thorough examination using density functional theory (DFT) and time-dependent (TD)-DFT to investigate the structural and optoelectronic properties of pentacene-based organic molecules (PbOMs) as potential donor material for organic photovoltaic BHJ devices. Our results show that oxadiazole prefers to attach via its nitrogen atoms to the carbon atoms of the pentacene monomer with an adsorption energy about − 32.86 kcal/mol, which means that oxadiazole is efficiently adsorbed on the edge of the pentacene. The HOMO energy level of the PbOM with the lowest bandgap is − 4.00 eV wide, i.e., about 0.86 eV lower and more positive than pentacene, thus providing an ideal open-circuit voltage for photovoltaic devices. The bandgap of the PbOM compounds are about 1.61 and 1.80 eV affording an efficient charge transfer from donor to acceptor. Furthermore, the donor PbOMs are also more stable than the pentacene. We have examined, additionally, the reactivity and absorption properties of individual molecules and PbOM systems. Our results suggest that the PbOM, as a donor material, may significantly improve the efficiency of BHJ solar cells.

Pentacene; Donor material; Bulk-heterojunction; TD-DFT.