Computational Investigation to Estimate the Electronic Properties of Polythiophene and Poly(3-butylthiophene-2,5-diyl) for High-Efficiency Solar Cells

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During the last decades, researchers were intensively studying and developing novel materials embedded in organic photovoltaic devices (OPVs), whose technology principle is to convert sunlight into electrical energy by using polymers. More precisely, donor-acceptor (DA) π-conjugated copolymers have been used for their harvesting photons efficiency due to their small optical gap, and for their electronic conductivity intrinsically produced by the concomitent presence of electron-donor and withdrawing groups. Searching for high-performance devices, it is also possible to widely tune the OPV active layer incorporating fullerenes as PC71BM and non-fullerene acceptors (NFAs) as O6T-4F, due to their important role on the exciton separation and electron transport of the material. This work aims to engineer OPVs combining NFAs and fullerenes into single covalent molecules. Here we report the first steps of this investigation using modelling to identify ideal molecules and predict their electronic properties. We employed Density Functional Theory (DFT) for studying a series of DA oligomers, doing a range of computational simulations to well-estimate energy levels and wavefunction behaviour.