Role of chlorine, bromine, iodine, and dehalogenation in the fluorinated small molecule Y6 for highly efficient organic solar cells.

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November 9, 2021

Abstract

In a recent experimental investigation, the chlorination of the highly efficient Y6 fluorinated molecule improved up to 16.5 \% the power conversion efficiency of an organic solar cell. To understand the better performance of BTP-4Cl:PBDB-TF acceptor-donor combination in comparison with BTP-4F:PBDB -TF in the newly reported organic solar cell, DFT calculations were performed in order to obtain a diversity of parameters related to molecular proper ties, such as electroacceptance, electron energy levels, absorption spectrum, charge mobility, and kinetics in exciton dissociation/recombination processes. Interestingly, chlorination improves charge mobility and the capacity to accept electrons. The binding energy is lower for the chlorinated than the fluorinated molecule, revealing an easier exciton cleavage in the former. Absorption spectra are in line with experimental ones, suggesting an ex cellent donor-acceptor complementarity. Additionally, novel molecules were proposed taking into account synthesized compounds, and the same parameters were analyzed. Results showed exciting behavior for the theoretically suggested compounds. Many properties were improved with the proposed molecules, which can also be exploited in solar photocells. Although it is a challenge to simulate/model a complete photoactive layer of an organic solar cell, it is proved through electronic structure calculations that the properties of the materials involved in the photovoltaic device can be obtained. In this way, give some light on the power conversion efficiency comparison and propose new compounds.

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