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Planarity and Multiple Components Promote Organic Photovoltaic Efficiency by Improving Electronic Transport

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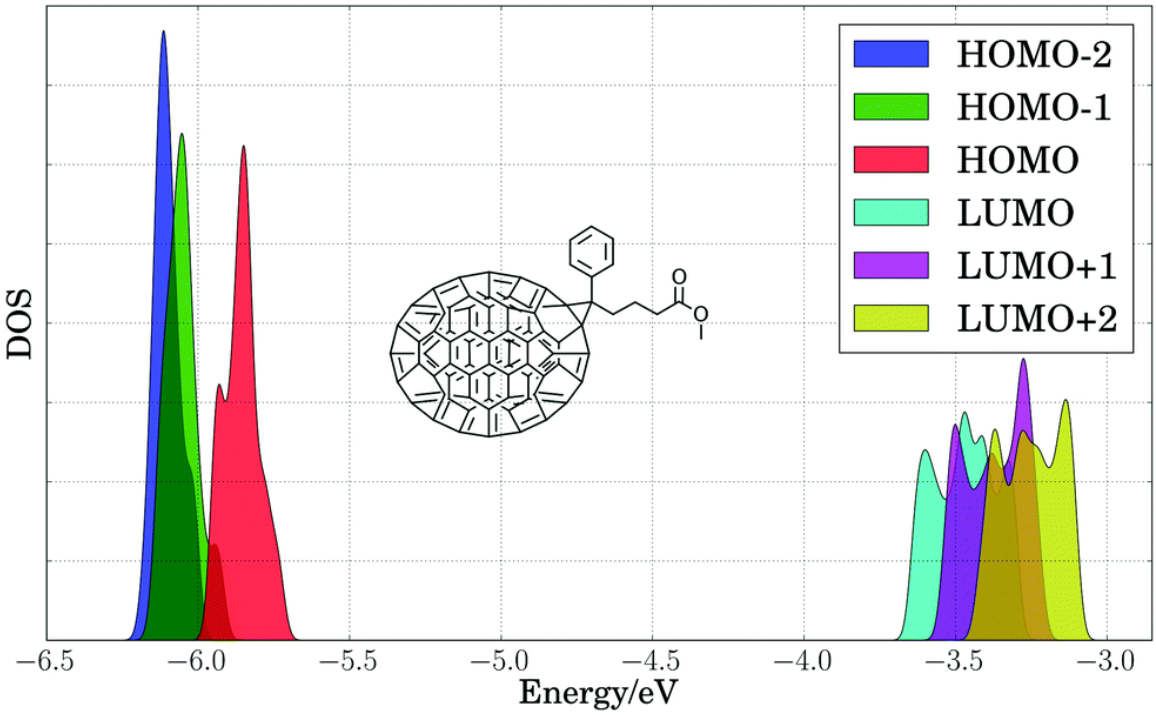

Caption: *Density of states (DOS) of calculated B3LYP HOMO−2, HOMO−1, HOMO, LUMO, LUMO+1, and LUMO+2 energy levels (eV) for 80 PC71BM configurations, with each energy level marked by color. A Gaussian broadening of 0.02 eV was applied to computed energy levels.*

Scientific Achievement

Establishing how the conformation of organic photovoltaic (OPV) polymers affects their electronic and transport properties is critical in order to determine design rules for new OPV materials and in particular to understand the performance enhancements recently reported for ternary blends. We report coupled classical and *ab initio* molecular dynamics simulations showing that polymer linkage twisting significantly reduces optical absorption efficiency, as well as hole transport rates in donor polymers. We predict that blends with components favoring planar geometries contribute to the enhancement of the overall efficiency of ternary OPVs. Furthermore, our electronic structure calculations for the PTB7–PID2–PC71BM system show that hole transfer rates are enhanced in ternary blends with respect to their binary counterpart.

Finally, our results point at thermal disorder in the blend as a key reason responsible for device voltage losses and at the need to carry out electronic structure calculations at finite temperature to reliably compare with experiments.

Significance

Through this work, we provide fundamental insight into voltage losses in polymer photovoltaic devices, attributing these partially to thermal disorder, an under-appreciated effect. Our results support the charge transport theories of our CHiMaD-funded collaborators as to one mechanism for non-linear gains in ternary OPV. Furthermore, we also found that intermolecular interactions between polymer components can result in favorable structural changes, increasing planarity and thus charge transport rates.

Citation

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