Organic Photovoltaics

Lightweight, abundant, cheap, environmentally-benign, flexible, and strongly absorbing, organic materials are promising for next-generation energy conversion applications. However, many organic-based solar energy conversion devices suffer from low efficiency and degradation. Improvement in either area relies on understanding the fundamental properties of these materials – and hybrid interfaces with other organics (e.g. donor-acceptor) and inorganics (e.g. metal contact or photoabsorbing semiconductor catalyst) – but is hindered by the challenges in characterizing their electronic structure, both experimentally and theoretically, at nanometer length scales.

Open-Circuit Voltage of Organic Photovoltaics

Alison Hatt posted on Apr 04, 2012

Optimizing open-circuit voltage (Voc) remains a significant challenge for organic photovoltaics (OPV). In OPVs, where small molecules or polymers comprise donor and acceptor, Voc depends largely on atomic-level details of the donor-acceptor interface. This dependence is not well understood, however, because interfacial energetics are extremely challenging to probe experimentally.

To address this problem, we use a parameter-free density functional theory-based method to get quantitative insight into the electronic structure and morphology of OPV donor-acceptor interfaces.

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