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Impact of Mesoscale Order on Energetics at Organic Donor-Acceptor Interfaces

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The interaction of charged excitations with the molecular surrounding in organic semiconductors is strictly long-ranged, due to their quadrupolar building blocks and preferential or absolute structural order. We show how atomistic simulations access the resulting energetics of charges and charge pairs and derived quantities, notably the charge-density-dependent open-circuit voltage across organic heterojunctions, with excellent accuracy. We compute level diagrams for a variety of donor-fullerene interfaces, with direct experimental validation, investigating relationships among photovoltaic gap, charge-transfer energetics and open-circuit voltage.

The underlying simulation approach takes into account long-range electrostatic effects that persist up to the mesoscale. The resulting mesoscale fields not only produce flat level profiles, but provide orientation-dependent push-out forces across a donor-acceptor interphase that can drive the charge-separation process. Correct polarity of these push-out forces is a requirement for functional solar cells, with operation closely above an isopolar point as the optimum tradeoff between magnitude of these push-out forces versus photovoltaic gap.

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