CT states in molecular blends: Interpretation of measured open circuit voltage and observed CT transitions with DFT-based calculations

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Charge transfer (CT) states around the donor-acceptor interface in an organic solar cell determine the device performance in terms of the open circuit voltage [1, 2]. Moreover, photovoltaic blends show weak absorption and electroluminescence features below the optical gap of the pure donor and acceptor materials, giving direct access to the spectroscopic impact of CT states. The application of computational schemes based on density functional theory (DFT) to CT energies have to circumvent spurious errors arising from the wrong asymptotics of standard exchange-correlation functionals. DFT with constraints guaranteeing the correct net charges on the ionized donor and acceptor molecules has shown promising results, indicating that the CT energies rely simply on the ionization potential of the donor and the electron affinity of the acceptor. Together with an embedding scheme accounting for the polarizable medium, the calculated CT energies agree reasonably well with the low-temperature limit of the open circuit voltage [3]. Calculated reorganization energies for the ionized molecules allow to interpret the observed Stokes shift and line broadening, demonstrating that the broad absorption and luminescence features are an intrinsic property of the CT state, not the result of an ensemble average [4].

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