Impact of the interfacial state's properties on organic solar cell performance

Solution processable molecular semiconductors are attractive for low-cost, low-embodied-energy solar cells. The advent of novel acceptor molecules propelled the power-conversion efficiencies of these devices to over 19%. This efficiency improvement is attributed to efficient charge generation even at low offset between the donor and acceptor molecular energy levels. The properties of the electronic state at the interface between the donor and acceptor molecular domains control both the charge generation and recombination. In this contribution, I present how we probe the properties of these excited states and model their impact on the device performance.

Electro- and photoluminescence have proved to be valuable tools to probe the energy and dynamics of excited states involved in photoinduced charge separation, and to identify structural and energetic disorder at molecular interfaces. Here, we use luminescence and other spectroscopic probes along with transient electrical measurements to study charge generation and photovoltage in molecular donor: acceptor solar cells. We then develop an integrated modelling framework in which excited state dynamics are combined with a one-dimensional device model that accounts for spatial variations in charge density. The integrated model allows different experimental measurements to be reconciled within a single picture and helps to show how the energies and dynamics of interfacial states influence the overall device performance. We use our results to consider the ultimate limitations placed on solar to electric conversion by the molecular nature of the materials.