

A single-molecule view of the structure and energetics at interfaces in dilute heterojunction organic solar cells

E. Mårzell^{1,2}, B. K. Yuan¹, K. A. Cochrane¹, M. D. DeJong¹, D. J. Jones¹, M. Riede³, and S. A. Burke¹

¹Stuart Blusson Quantum Matter Institute, University of British Columbia, 2355 East Mall, Vancouver, BC V6T 1Z4, Canada.

²Division of Molecular and Condensed Matter Physics, Department of Physics and Astronomy, Uppsala University, Box 516, 751 20 Uppsala, Sweden.

³Clarendon Laboratory, Department of Physics, University of Oxford, Oxford OX1 3PU, England, UK.

Organic photovoltaics offers a path to lightweight, flexible, and low-cost solar cells, but suffers from low power conversion efficiencies. This is partly because of a tradeoff between open circuit voltage and generation efficiency of free charge carriers. The active region in an organic solar cell typically consists of a blend layer of roughly equal amounts of donor and acceptor molecules, where the interface facilitates dissociation of the strongly bound exciton into separated charges. Recently, it was shown that reducing the donor concentration in bulk heterojunction solar cells to 5–10% can improve the open circuit voltage by more than 100 mV, resulting in an improved power conversion efficiency in these systems [1]. Questions however remain about the energetics of the interface and how it correlates with light absorption and exciton dissociation in these almost single-component solar cells.

To study the heterojunction interface in detail, we use a combination of low-temperature scanning probe microscopy techniques applied to model systems of such dilute heterojunctions. The model systems consist of single impurity molecules on multilayer C60 films deposited *in situ* in an ultrahigh vacuum chamber. This gives us access to a controlled system where we can study the interface with sub-molecular spatial resolution. As model impurity molecules, we choose zinc phthalocyanine (ZnPc) functionalized with different amounts of fluorine, as these molecules are structurally similar but display different energy level alignments [2].

The physical structure of the system is measured using atomic force microscopy with a CO-functionalized tip for submolecular resolution. The electronic structure is instead measured using pixel-by-pixel scanning tunnelling spectroscopy (STS) to reveal the local density of states. We show how the different impurity molecules affect the energy levels of the surrounding C60 molecules on a nanometre scale.

[1] M. Zhang *et al.*, *Adv. Mater.* **23**, 4960 (2011).

[2] M. Schwarze *et al.*, *Science* **352**, 1446 (2016).