Fonda-Fasella award presentation

Understanding energy level alignment in donor-acceptor/metal interfaces

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Charge carrier injection in organic optoelectronic devices depends on the electronic properties of metal/organic interfaces, which are therefore of utmost importance for the device efficiency. That interface can be generally defined by a monolayer-thick blend of donor and/or acceptor molecules in contact with a metal surface. Energy barriers for electron and hole injection are determined by the offset from HOMO (highest occupied) and LUMO (lowest unoccupied) molecular levels of this contact layer with respect to the Fermi level of the metal electrode. However, the HOMO and LUMO alignment is often not easy to elucidate in complex multi-component, molecule/metal systems. Here we demonstrate that core-level photoemission from donor-acceptor/metal interfaces can also be used in the assessment of molecular level alignment. Systematic experiments in a variety of model systems show a characteristic binding energy shift in core-levels as a function of molecular donor/acceptor ratio, irrespectively of the molecules or the metal. Such shift shows that the electronic properties of metal-organic interfaces measured on single-component layers cannot be naively extrapolated to the new supramolecular environment of donor-acceptor molecular blends. Instead, it reveals how the level alignment at the molecule/metal interface varies according to the donor-acceptor stoichiometry-dependent work function of the molecular blends.