

# Energy Level Alignment at Weakly-Interacting Organic/Metal and Organic/Organic Interfaces: The Integer Charge Transfer Model

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## Abstract

The fundamentals of energy level alignment in organic electronics are described. We focus on weakly-interacting organic/metal and organic/organic interfaces that are formed under ambient conditions, for example by solution processing of polymers, or, more generally, when the substrates are passivated by oxides or residual hydrocarbons. The resulting decoupling of the  $\pi$ -electrons from the substrate bands/orbitals prevents hybridization of electronic states, and consequently blocks the formation of interface dipoles via partial electron transfer. In many cases, it has indeed been shown that there is no vacuum level shift at such interfaces. However, electron transfer can still occur via tunnelling, and does occur when the substrate work function is higher (lower) than the formation energy of positively (negatively) charged states in the organic material [1,2]. Tunnelling implies the transfer of an integer amount of charge, one electron at a time, into well defined charged states on the polymer or molecule, which becomes energetically allowed under the conditions mentioned. Hence, a sharp transition between a vacuum level alignment regime and a Fermi level pinning regime occurs as the substrate work function crosses the threshold value. The nature of the integer charge transfer levels depends on the materials system: for conjugated large molecules and polymers, the integer charge transfer states are polarons or bipolarons, for small molecules, highest occupied and lowest unoccupied molecular orbitals, though in the latter case Coulomb-Coulomb repulsion may significantly distort the molecular orbital energy upon addition of an extra electron. In all cases, the integer charge transfer states are affected by the substrate “mirror” charge, significantly shifting their formation energy from the corresponding bulk values. The Integer Charge Transfer model [1,2] for weakly-interacting interfaces is illustrated with experimental results on polymer/metal, molecule/metal, polymer/polymer and molecule/polymer interfaces. Finally, limits and further improvements to the Integer Charge Transfer model are discussed as well as impact on device design.

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2. M. Fahlman, A. Crispin, X. Crispin, S.K.M. Henze, M.P. de Jong, W. Osikowicz, C. Tengstedt and W.R. Salaneck: *J. Phys.: Condens. Matter* **19** (2007) 183202.