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Charge transfer and polarization at interfaces with conjugated molecules

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The function and efficiency of organic electronic devices is determined to a significant extent by the electronic properties of organic/organic heterojunctions and interfaces between electrodes and organic semiconductors. The energy level alignment between metal electrodes and active organic layers can be adjusted over wide ranges by employing interlayers of strong molecular acceptors and donors that undergo charge transfer reactions with the metal. It will be shown that such interlayers lead to lower charge injection barriers than pristine metals, even when the work function is the same. It is argued that the molecularly modified electrodes are electronically more rigid than their pristine metal counterparts, i.e., the electron spill-out at the organic-terminated surface is less pronounced compared to metal surfaces. The energy levels at organic/organic heterojunctions comprising donors and acceptors as used in organic photovoltaic cells are essentially independent of deposition sequence, as long as supporting electrodes do not induce energy level pinning. When a high work function electrode is used, the energy levels may become Fermi-level pinned and an electric field drops right at the heterojunction. This effect is exemplified for the donor diindenoperylene and the acceptor C60. The electric field distribution within an organic optoelectronic device may thus be adjusted locally by employing interfacial energy level pinning, even at weakly interacting organic/organic interfaces.