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Tailoring interface energy levels with molecular acceptors, donors, and switches: relevance for opto-electronic devices

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The electronic structure at interfaces determines the function and efficiency of electronic and opto-electronic devices, such as field effect transistors, light emitting diodes, and photovoltaic cells. Particularly the line-up of the frontier energy levels at heterojunctions is of interest and needs to be optimized with respect to the demands of the application. Regarding the interfaces between organic semiconductors and electrodes, the use of interfacial layers (in the monolayer regime) comprising strong molecular electron acceptors and donors turns out to be most versatile. The fundamental interactions and mechanisms that lead to a work function modification of electrodes (such as transparent conductive oxides and polymers, metals, graphene) and the subsequent re-alignment of the organic semiconductor energy levels will be discussed. The experimental results are mostly obtained with photoemission spectroscopy. Overall, this concept allows spanning a work function range from below 3 eV to above 6 eV with one given electrode material. In turn, the level alignment of most organic semiconductors can thus be tailored to any value within the energy gap.

While the above method is static, i.e., set by the employed molecular layers, the use of photochromic molecular switches enables a dynamic character of the interface electronic properties. By simple optical stimulus, molecular switches provide for a transient electronic density of states at interfaces, which has a huge impact on charge injection and transport in conjunction with organic semiconductors.