

Modelling the electronic properties of metal-organic interfaces

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During the past years, the crucial role of interfaces in organic (opto)electronic devices has been increasingly acknowledged. This calls for strategies for controlling their properties. Two particularly promising approaches are the use of functional self-assembled monolayers (SAMs) and charge transfer monolayers. Both allow tuning electrode work functions and especially SAMs are promising for applications in molecular electronic devices. In the present contribution, fundamental concepts for how such functional layers influence interface properties will be discussed using density-functional theory based band-structure calculations.^{[1],[2]} In this context, the focus will lie on understanding the relationship between the chemical structure of the used molecules and the achieved work-function modification and energy-level alignment. For SAMs, we will discuss, how these properties are affected by changing head-group substituents,^[3] the molecular backbone^{[4],[5]} and the docking group,^[6] the consequences of distributing molecular dipoles along the molecules^[7] will be discussed and it will be addressed to what extent and under which circumstances SAM-induced work-function modifications translate into changes of the carrier injection barriers.^[8] For charge-transfer monolayers, it will be shown how donor (acceptor) molecules can be used to decrease (increase) electrode work-functions^{[9],[10],[11]} by a subtle interplay between charge forward and backward transfer processes in different parts of the molecule combined with intrinsic molecular dipole resulting from adsorption induced changes of the molecular geometry.

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