Pinning Effects at Hybrid Interfaces : A Theoretical Insight

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Molecules covalently attached to substrates play a pivotal role in nanoelectronics, in particular for the development of smart surfaces or molecular junctions. The energy level alignment between the molecular levels and the density of states of the substrate dictates the electronic properties of self-assembled monolayers and the amplitude of the current flowing across junctions. The molecular levels are typically broadened upon adsorption and shifted in energies due to interfacial charge redistribution processes. The conventional wisdom suggests that the alignment can be fine tuned by adding electroactive substituents on a given molecular backbone or by increasing the size of the conjugated path. However, several of our recent theoretical studies have evidenced strong pinning effects implying that the alignment can be insensitive to such chemical derivatizations. This has strong implications in many research areas since any molecular design performed in solution can be ruined when attaching molecules to the substrate. In this presentation, we will illustrate such pinning effects in several situations : (i) dye adsorbed on a TiO2 substrate in the field of dye-sensitized solar cells [1]; (ii) conjugated backbones of increasing size or with different substituents attached to a gold electrode [2,3]; and (iii) photochromic molecules inserted into molecular junctions [4,5].

References

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[4] C.Van Dyck et al. Physical Chemistry Chemical Physics 15 (2013) 4392-4404.

[5[C.Van Dyck et al. Advanced Functional Materials 24 (2014) 6154-6165.

Figure

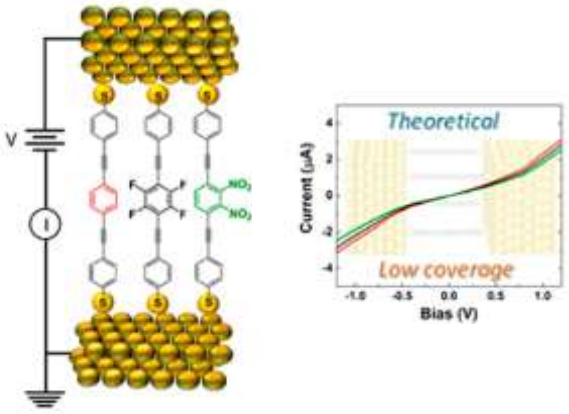

Figure 1: Illustration of the pinning effects in molecular junctions