

Electron and spin transport through hybrid organic-inorganic interfaces and in molecular devices: insights from first-principles and model calculations

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The field of molecular spintronics has developed along two complementary paths. On the one hand, a large research effort has been dedicated to the study of the interfaces between molecules and ferromagnetic metals in order to understand how their electronic structure influences spin-injection and spin-transport in hybrid organic-inorganic spin-valve devices [1]. On the other hand, many studies have investigated whether a single molecular spin can be addressed in molecular transistors. We here, present several results, which provide a contribution to both research directions.

In the first part, we describe, from a theoretical perspective, how spin-polarized hybrid interface states affect the electron tunneling through organic-inorganic interfaces. However, we also show that, for diffusive transport, these hybrid states are less important. In contrast, in this case, electrons can be trapped in the first few organic layers near the interface, while they undergo an electron-vibron driven spin-relaxation. Our results, which have been obtained by a combination of density functional theory and model calculations, rationalize recent experimental observations [2] and suggest that spin-relaxation effects at hybrid interfaces may hinder spin-transport in spin-valve devices.

In the second part, after briefly presenting our implementation of the dynamical mean-field theory [3] in the Smeagol transport software [4], we discuss how material specific properties affect the nature of the Kondo effect in molecular devices. In particular, we show that the Kondo effect, besides being a tool to characterize the spin of a molecule, may be utilized in order to infer many other information about a molecular device (e.g. the most-likely molecule absorption site or the molecular conformation). A selected example of electron transport through radical molecules is presented.

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References

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