Electronic structure influence on the conductivity through open- and closed-shell molecules

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Molecular Spin Electronics or *Molecular Spintronics*[1] is a novel field in which the effort is being placed on exploring the spin transport properties of organic systems (i.e. spin injection and spin conservation). Its high potential in applications such as novel spin-based magnetic recording and memory devices has recently aroused high attention.

Our study relies on the transport properties comparison between two self-assembled monolayers (SAMs) based on polychlorinated triphenylmethyl (PTM) derivatives, in the radical (magnetic) and non radical (diamagnetic) form. These SAMs exhibit small differences in their molecular structure but strongly differ in their electronic configuration (closed and open-shell forms). The investigation of the transport properties was performed by the so-called 3D operation mode of C-SFM. Similar measurements were carried out on SAMs prepared following two different approaches. In the first one, PTM molecules were grafted to a gold surface which was previously modified[2] and second, a novel PTM molecule was designed to be anchored to the Au in one step leading to a fully conjugated system bonded to the surface thus, resulting in a larger hybridization of the molecules with the metal (Figure 1).[3] In both cases the open-shell form resulted being significantly more conducting. By density functional calculations, this observation was suggested to occur due to a single-unoccupaied orbital (SOMO) mediated transport in the case of the open-shell system. Interestingly, at larger bias applied negative differential resistance (NDR) was observed for the fully conjugated closed- and open-shell SAMs (Figure 1).[3] The fact that the LUMO energy level of non-radical PTM is close to the LUMO-α of radical PTM suggests that if a high negative voltage is applied to the tip shifting upwards its work function, resonant conduction through these unoccupied orbitals could take place in both SAMs. Such an effect could account for the NDR peaks. The observation of NDR could be used to perform logic and memory functions in electronic circuits.[4]

References

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Figures

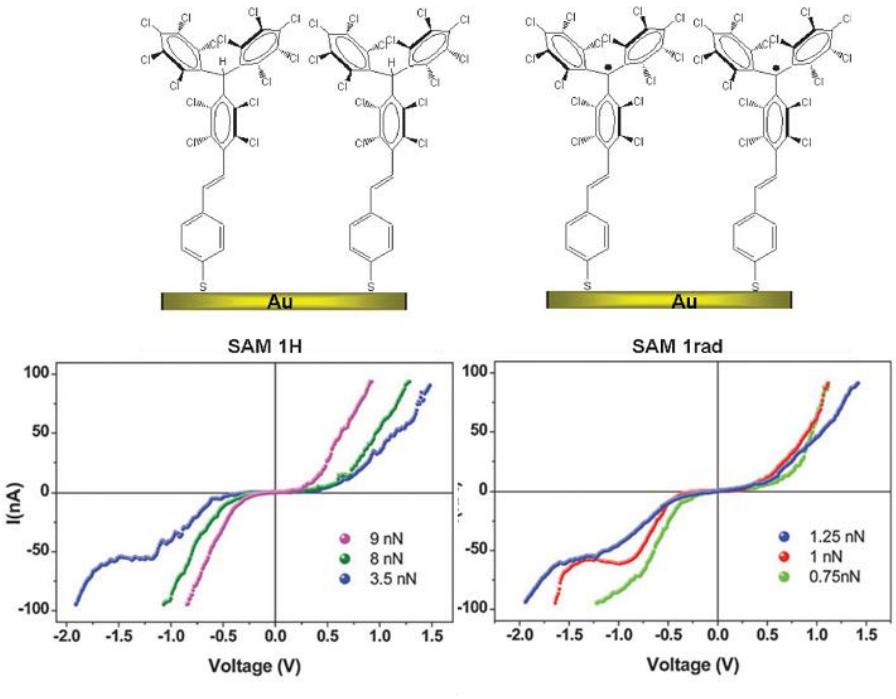

Figure 1. Scheme of the fully conjugated open (SAM 1rad) and closed-shell (SAM 1H) PTM SAMs and their corresponding *I*–*V* curves as a function of the applied load.