

## Inducing new molecular properties at the metallic interface

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The electronic and magnetic properties of organic compounds are in most cases strongly modified by the presence of a metallic interface [1]. The dramatic effect of the bonding configuration at the interface is in fact the responsible for the lack of reproducibility in the transport properties of molecular junctions [2]. On the other hand the metallic interface offers the possibility to induce new molecular charge and spin configurations. Understanding the correlation between conformational and spectroscopic properties at the atomic scale is therefore fundamental to control the properties of molecular junctions, and the STM represents an ideal tool for such investigation.

Here we show how a careful choice of molecule-metal interaction can lead to interesting phenomena such as the induction of chiral molecular orbitals in achiral molecules [3], and of magnetism in organic compounds [4]. Using single metal-phthalocyanines deposited on Ag(100), we see that both effects depend on the central metal ion, which determines the active orbitals [5]. In the case of spin induction, the spatial localization of the Kondo resonance we observe indicates that the new spin belongs to a ligand orbital and coexists with that of the central transition metal ion. Magnetic excitations of the coupled spins contribute to the inelastic tunnelling, from which we can determine the magnetic ground state and intramolecular exchange coupling energy. Finally, we explore several methods to manipulate the charge and spin configuration by moving individual molecules in order to form intermolecular bonds or alkali atoms to electron-dope the molecules [6]. Atom by atom doping results in a manifold of charge and spin configurations, where the amount of charge is controlled by the dual donor/acceptor capability of the substrate and its localization in metal or ligand orbitals depends on the bonding site. The presented results highlight the need of considering the molecule-metal interface as a functional, active part of molecular junctions.

[1] S. Sanvito, Chem. Soc. Rev. 40, 3336 (2011).

[2] L. Bogani and W. Wernsdorfer, Nat. Mater. 7, 179 (2008).

[3] A. Mugarza et al., Phys. Rev. Lett. 105, 115702 (2010).

[4] A. Mugarza et al., Nature Comm. 2:490 (2011).

[5] A. Mugarza et al., Phys. Rev. B 85, 155437 (2012).

[6] C. Krull et al., Nature Mater. 12, 337 (2013).