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TÉMA

Electronic and magnetic properties of supported transition metal phthalocyanines

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Advances in the development of molecular devices depend on the ability to control the charge and spin of single individual molecules at the interface with a metal. By density functional theory calculations and scanning tunneling spectroscopy experiments we have investigated the molecule-surface interactions of supported transition-metal phthalocyanines. We have studied how charge transfer and spin moment change by hybridization with the surface, and as a function of the occupancy of the *3d* metal states. We discuss the utility of the anion as a model of the supported situation, and we analyze the results regarding the Kondo effect observed in some situations.

We also show that doping of individual molecules by alkali atoms can be used to individually change the molecular spin. Furthermore, a scanning tunneling microscope can be used to place or remove the spin dopant on the molecule, allowing us to manipulate the spin of an individual molecule in a controlled way. The comparison between conductance measurements and density functional theory calculations allows us to gain deeper insight into the doping mechanism.

[1] A. Mugarza et al, Nature Communications 2, 490 (2011).
[2] A. Mugarza et al, Physical Review B 85, 155437 (2012).
[3] R. Robles et al, Nano Letters 12, 3609 (2012).

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