Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

August 28th 2014 – 11:00

CFEL Seminar room V, 01.109 (Bldg. 99)

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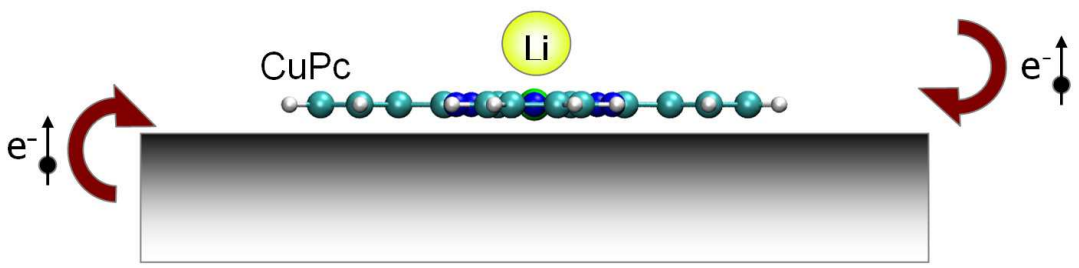
Site- and orbital-dependent charge and spin manipulation in supported transition metal phthalocyanines

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. Chemical doping is one promising way of achieving this goal, but its usefulness depends on the ability to understand the interplay between dopants, molecules and metallic surfaces. Here we use scanning tunneling microscopy experiments and electronic structure calculations to investigate the doping of supported transition-metal phthalocyanines by alkali atoms. We study 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 show how the doping of individual molecules by alkali atoms can be used to individually change the molecular charge and spin. Furthermore, a scanning tunneling microscope can be used to place dopants on the molecules with intraatomic resolution, allowing us to identify at least three stable adsorption sites, and to manipulate the spin of an individual molecule in a controlled way without resorting to the use of magnetic dopants. 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] C. Krull et al, Nature Materials 12, 337 (2013).



Host: Sebastian Loth

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