

Many-body transitions in a single molecule visualized by scanning tunneling microscopy

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Scanning tunneling spectroscopy (STS) of molecular systems is usually interpreted in terms of single-particle electronic transitions [1]. A prominent exception is the Kondo effect [2], a many-body state resulting from the interaction of an unpaired molecular spin with the conduction electrons of a metallic substrate. However, the Kondo effect is a property of the coupled molecule-substrate system and does not correspond to an intrinsic many-body state of the molecule. Probing excited states in single molecules by STS, we demonstrate many-body effects arising purely from electronic states confined in the molecule.

Cobalt phthalocyanine (CoPC) molecules deposited onto monolayer hexagonal boron nitride (h-BN) on Ir(111) [3] allows to carry out STS on molecules that are initially in different charge states [4]: A moiré superstructure formed by h-BN on Ir(111) results in a periodic modulation of the local work function and CoPC adsorbing either in a neutral or negatively charged ground state. The observed molecular resonances are inconsistent with the single-particle interpretation of tunneling spectroscopy. Instead, combining time-dependent density functional theory calculations with STS wave function maps, we show that they can be understood as a series of many-body excitations of the different ground states of the molecule [5].

[1] F. Albrecht et al., *J. Am. Chem. Soc.* **135**, 9200 (2013).

[2] I. Fernandez-Torrente et al., *Phys. Rev. Lett.* **101**, 217203 (2008).

[3] F. Schulz et al., *Phys. Rev. B* **89**, 235429 (2014).

[4] F. Schulz et al., *ACS Nano* **7**, 11121 (2013).

[5] F. Schulz et al., *Nature Phys.* **11**, 229 (2015).