A new view on the origin of zero-bias anomalies of Co atoms atop noble metal surfaces

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Many-body phenomena are paramount in physics. In condensed matter, their hallmark is considerable on a wide range of material characteristics spanning electronic, magnetic, thermodynamic and transport properties. They potentially imprint non-trivial signatures in spectroscopic measurements, such as those assigned to Kondo, excitonic and polaronic features, whose emergence depends on the involved degrees of freedom. With the help of scanning tunneling microscopy (STM), zero-bias anomalies assigned to be Kondo features were identified early on in Co adatoms on Au(111) surface [1]. This gave birth to a very active and exciting research field devoted to Kondo physics on surfaces that led to tremendous theoretical and experimental developments and discoveries.

In this talk, I will present our recent work [2] based on time-dependent density functional and many-body perturbation theories accounting for spin-orbit coupling. After a systematic first-principles investigation of Co adatoms on Cu, Ag and Au substrates, we find zero-bias anomalies quasi-identical to those measured by STM. The obtained features originate, however, from gaped spin-excitations induced by a finite magnetic anisotropy energy (MAE) in contrast to the usual widespread interpretation. Furthermore, we unveil a new many-body feature, the spinaron, resulting from the interaction of electrons and spin-excitations. I will show ways of reducing the MAE, for example by attaching Co atoms to Cu-wires, which enable easier magnetic-field measurements of the transport anomalies. Finally, I will address unconventional spin-excitations [3] before giving an overview of potential future experimental and theoretical investigations.

[1] Madhavan, Chen, Jamneala, Crommie, Wingreen, Science 280, 567 (1998)
[2] Bouaziz, Guimarães, Lounis, Nature Communications 11, 6112 (2020)
[3] Küster, Montero, Guimarães, Brinker, Lounis, Parkin, Sessi, Nature Communications 12, 1108 (2021)