

Interplay between Kondo effect and molecular quenching in magnetic molecules at metal substrates from first principles

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When a magnetic molecule is deposited on a metallic substrate or attached to metal leads, the Kondo effect can take place, thereby screening its magnetic moment. On the other hand strong coupling of the transition metal center to the organic ligands also leads to quenching of the spin. Using our DFT based ab initio approach for nanoscale devices explicitly taking into account the dynamic correlations originating from strong electronic interactions [1,2], we calculate the electronic structure and STM spectra of high spin complexes on metal surfaces. Our calculations reveal the complex interplay of the Kondo effect and molecular quenching processes in these systems. Furthermore we find that Kondo screening via the organic ligands leads to novel features in the spectral function near the Fermi level different from the usual Kondo peaks [3].

[1] D. Jacob, K. Haule and G. Kotliar, PRL 103, 016803 (2009)

[2] M. Karolak, D. Jacob and A. I. Lichtenstein, PRL 107, 146604 (2011)

[3] D. Jacob, M. Soriano and J.J. Palacios, PRB 88, 134417 (2013)