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A fully firstprinciples approach to the molecular Kondo problem
MARA SORIANO, JUAN JOS PALACIOS, Univ Autonoma de Madrid, DAVID JACOB, Max-Planck-Institut Mikrostrukturphysik — There has been a great effort in recent years to understand the emerging Kondo-like resonances in different magnetic molecules such as MnPc. Theoretical approaches based on atomic models have proven to be very useful for the study of this phenomenon when the magnetic moment is essentially localized on a magnetic atom [1,2]. Nevertheless the Kondo effect can arise in pure carbon-based systems as has been demonstrated experimentally in fullerenes and carbon nanotubes [3]. In this communication we present a fully first principles approach to the molecular Kondo problem based in a combination of atomistic calculation and a multiorbital Anderson model where the orbitals are not atomic but molecular orbitals. That allows us to address this problem in systems with delocalized spin states, such as fullerenes, and in general in all kind of organic molecules such as radicals, where the atomic and conventional models fail. This model is fully obtained from Density Functional Theory calculation in combination with Green's functions methodologies [4,5]. [1] Phys. Rev. Lett. 109, 147202 (2012); [2] Phys. Rev. B 88, 134417 (2013); [3] Nature 434, 484. (2005); [4] ANT.G03. www.alacant.dfa.ua.es; [5] Phys. Rev. B. 82, 195115 (2010).

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