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A fully first-principles approach to the Molecular Kondo problem MARIA SORIANO, Univ Autonoma de Madrid, DAVID JACOB, Max Planck Institute of Microstructure Physics, JUAN JOSÉ PALACIOS, Univ Autonoma de Madrid, ATOMELIX TEAM — 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 [3,4]. In this communication we present a multiorbital Anderson model where the orbitals are not atomic but molecular orbitals. This model is fully obtained from Density Functional Theory calculation in combination with Green's functions methodologies [5,6]. Standard impurity solver techniques are used to solve the model which is applied to fullerenes and other nanographene structures [7].

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