Abstract Submitted for the MAR14 Meeting of The American Physical Society

A molecular approach to the Kondo problem in Carbon based systems MARIA SORIANO, Universidad Autonoma de Madrid, Madrid, Spain, DAVID JACOB, Max-Planck-Institut fur Mikrostrukturphysik, Halle (Saale), Germany, JUAN JOSE PALACIOS, Universidad Autonoma de Madrid, Madrid, Spain — There has been a great effort in recent years to understand the emerging Kondolike 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].

- [1] A. Strózecka et. al. Phys. Rev. Lett. 109, 147202 (2012);
- [2] D. Jacob et. al. Phys. Rev. B 88, 134417 (2013);
- [3] J. J. Parks et. al. Phys. Rev. Lett. 99, 026601 (2007);
- [4] P. Jarillo-Herrero et. al. Nature 434, 484. (2005);
- [5] ANT.G03. www.alacant.dfa.ua.es;
- [6] D. Jacob et. al. Phys. Rev. B. 82, 195115 (2010);
- [7] J Fernandez-Rossier et. al. Phys. Rev. Lett. 99, 177204 (2007).

Maria Soriano Universidad Autonoma de Madrid

Date submitted: 15 Nov 2013

Electronic form version 1.4