# Spin and Orbital Magnetism of Rare Earth Atoms Adsorbed on Graphene and Metal Substrates

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Surface supported single magnetic atoms, the so-called "single-atom magnets", open new opportunities in a quest for the ultimate size limit of magnetic information storage. Initially, the research mainly focused on 3d-atoms on surfaces, but none of them were found magnetically stable above 0.3 K. Very recently, the attention was turned to the rare-earth (RE) atoms, culminating in the experimental discovery of magnetically stable Ho atom on MgO(001) substrate [1], and Dy atom on graphene/Ir(111)[2].

I address the electronic and magnetic character of RE atoms on a free-standing graphene (Gr), and Pt(111) substrate making use of the methods beyond the conventional density functional theory (DFT+U, and DFT+"Exact Diagonalization" (ED)). The DFT+U method predicts for Sm@Gr atom to carry local magnetic moments (spin and orbital) contrary to a non-magnetic, J=0 ground-state configuration of Sm in the gas phase. Application of DFT+ED method cures this problem, and yields a non-magnetic ground state with six f electrons and J=0 [3]. The spin and orbital magnetic moments of Ho@Pt(111) are evaluated [4] and compared with experimental X-ray magnetic circular dichroism (XMCD) data. The magnetic anisotropy energy is estimated, and the magnetic stability is discussed. The role of 5d-4f interorbital exchange polarization in modification of the 4f-shell energy spectrum is emphasized.

[1] F. Donati et al., Science 352, 318 (2016).
[2] R. Baltic et al., Nano Lett. 16, 7610 (2016).
[3] A. Kozub, A. B. Shick, F. Maca et al., Phys. Rev. B 94, 125113 (2016).
[4] A. B. Shick, D. S. Shapiro, J. Kolorenc, A. I. Lichtenstein, Sci. Rep. 7, 2751 (2017).