European XFEL Theory Seminar

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Campus Schenefeld, main building (XHQ) room E1.096

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Electronic and magnetic character of rare-earth adatoms on graphene and platinum surface

The electronic structure of selected rare-earth atoms adsorbed on a free-standing graphene (Sm@Gr) and platinum (111) surface (Ho@Pt(111)) was investigated using the methods beyond the conventional density functional theory (DFT+U, and DFT+Exact Diagonalization (ED)). The influence of the electron correlations and the spin-orbit coupling on the magnetic properties was examined. 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.

For Ho@Pt(111), paramagnetic DFT+ED calculations result in $\langle J_z \rangle = 0$, double-degenerate ground state $|J=8, J_z=+/-\ 8\rangle$. When the system is magnetized by the external magnetic field, the ground state transformes to $\langle J_z \rangle = 6.6$ magneticaly polarized state. It is shown that DFT+ED results are in better agreement with recent XMCD experimental data [1] than previously reported DFT+U calculations [2]. The role of *5d-4f* inter-orbital exchange polarization in modification of the Ho *4f*-shell energy spectrum is emphasized. Our findings can play an important role in quantitative theory of recently discovered single atom/molecule magnets [3].

[1] F. Donati *et al.*, Phys. Rev. Lett. 113, 237201 (2014).

[2] J. H. Miyamachi *et al.*, Nature **503**, 242 (2013).

[3] F. Donati *et al.*, Science **352**, 318 (2016).

Host: Evgeny Gorelov