Many-body models for molecular nanomagnets

Eva Pavarini

Institute for Advanced Simulation and JARA High-Performance Computing

I will present a novel [1] flexible and effective scheme to build *ab-initio* many-body models –and the corresponding low-energy magnetic Hamiltonians– for molecular nanomagnets. It is based on using localized Foster-Boys orbitals as a one-electron basis. I will illustrate applications of this scheme to some paradigmatic systems: the antiferromagnetic rings Cr_8 and Cr_7 Ni, the single-molecule magnet Fe_4, and two Cr_7Ni-Ni-Cr_7Ni assemblies [1,2].

[1] A. Chiesa, S. Carretta, P. Santini, G. Amoretti, and E. Pavarini,
Phys. Rev. Lett. **110**, 157204 (2013).

[2] A. Chiesa, G. Whitehead, S. Carretta, L. Carthy, G. Timco, S. Teat, G. Amoretti,
E. Pavarini, R. Winpenny, and P. Santini, Scientific Reports, in press (2014).