MAR08-2007-007458

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

**Magnetic ground state of small nanoparticles: Cr trimers on Au(111)**[1]

BALAZS UJFALUSSY, Research Institute for Solid State Physics

The development of scanning tunneling microscopy (STM) and the ability to build clusters with well-controlled structures permit the study of various effects induced by local interactions within magnetic nanoclusters. However, for a clear interpretation of experimental results, first principles studies are often required, even when they are sometimes too demanding. In this talk we show a new way to map the energy of supported magnetic nanoparticles obtained from first principles calculations onto a classical spin Hamiltonian. The half-filled valence configuration of Cr yields a large magnetic moment and strong antiferromagnetic inter-atomic bonding leads in turn to magnetic frustration and complex spin phenomena. The simplest system exhibiting such properties is a trimer. The electronic structure of the Cr trimers are calculated by means of a fully relativistic Green's function embedding method. The relativistic treatment of the electronic structure leads to a proper account of spin-orbit coupling giving rise to tensorial exchange interactions and magnetic anisotropies influencing the formation of non-collinear ground states. In additon, we show that the inclusion of fourth-order terms into the spin-model largely enhance the accuracy of the mapping. The magnetic ground-state of the trimers are found as the solution of the Landau-Lifshitz-Gilbert equations. In case of an equilateral Cr trimer we show that the Dzaloshinsky-Moriya interactions lift the degeneracy of the 120° Néel states with different chirality. For the linear and the isosceles Cr trimers we obtain collinear antiferromagnetic ground states. We also address the issue of choosing the reference state inherent to methods based on the magnetic force theorem in the context to the equilateral Cr trimer. This freedom of the method might cause an ambiguity in determining the magnetic ground state of systems exhibiting metastable states close to the ground state.

[1]Work supported in part by the Division of Material Science and Engineering US-DOE and by the Hungarian government (contracts OTKA 68312 and F68726).