Chern-number spin Hamiltonians for magnetic clusters by ab-initio methods

Carlo M. CANALI
University of Kalmar
Division of Physics
Department of Chemistry & Biomedical Sciences
Nygatan 30, 391 82 Kalmar, Sweden

Abstract:

Combining field-theory methods and ab-initio calculations, we construct an effective Hamiltonian with a single giant-spin degree of freedom, capable of describing the low-energy spin dynamics of ferromagnetic metal nanoclusters consisting of up to a few tens of atoms. In our procedure, the magnetic moment direction of the Kohn-Sham spin-density functional theory wave-function is constrained by means of a penalty functional, allowing us to explore the entire parameter space of directions, and extract the magnetic anisotropy energy and the Berry curvature functionals. The average of the Berry curvature over all magnetization directions is a so-called Chern number, a topological invariant that can only take on values equal to multiples of half-integers, which represents the dimension of the Hilbert space of the effective spin system. The spin Hamiltonian is obtained by quantizing the classical anisotropy-energy functional, after a change of variables to a constant Berry-curvature space. We illustrate this procedure by explicitly constructing the Hamiltonian for dimers and trimers of transition-metal atoms, whose spin dynamics has been recently investigated experimentally by STM methods.

[Work done in collaboration with T.O. Strandberg and A.H. MacDonald]