MAR06-2005-006011

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Density-Functional Theory of Molecular Magnets[1]

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Molecular magnets are large (a few nanometers in diameter), well-defined, discrete molecules consisting of several transition metal ions interacting through organic and/or inorganic ligands. Among thousands of synthesized molecular magnets, there is a class of molecular magnets known as single-molecule magnets (SMMs) which have large effective magnetic moments and behave as single-domain magnetic nanoparticles in an external magnetic field. They are particularly interesting because of observed quantum tunneling of magnetization and their possible applications in magnetic recording and molecular electronics. In this talk, I will demonstrate how quantum mechanics can be used to study the properties of SMMs from a first-principles vantage point. In particular, I will present density-functional calculations of the electronic, vibrational, and magnetic properties of selected SMMs, such as the total magnetic moment, electronic energy gaps, Raman scattering spectra, exchange constants, spin excitation energetics, and magnetic anisotropy barriers. I will also discuss what types of molecular environmental changes can significantly influence the exchange interaction, magnetic anisotropy, and observed quantum tunneling in the SMMs.

[1]supported by the ONR, the DoD HPC CHSSI program, and the W.M. Keck Foundation