University of Minnesota
Driven to Discover℠

Department of Chemistry

Seminar

4 p.m. Monday, April 16 • 331 Smith Hall

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DFT-Based Simulation of Molecular Magnets

Research interests concentrate on the development, testing, and application of massively parallel electronic structure methods for the density-functional-based simulation of molecules and clusters.s.

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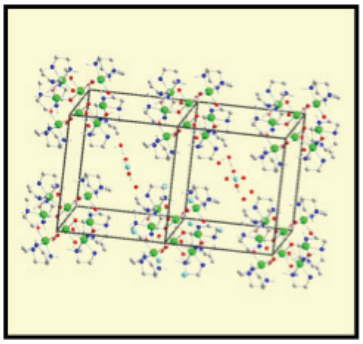
Abstract

The field of molecular magnetism began in the 1980s with the successful inorganic synthesis and subsequent crystallization of a new class of molecules composed of a collection of six-fold exchange-coupled transition-metal centers held in place by ligands. After experimental observations of long-lived magnetic bistability and collective quantum-mechanical magnetic behaviors (1993-1996), interest in this field grew significantly and it now includes an interdisciplinary mix of inorganic-, organic- and physical chemists as well as electronic-structure theorists, and many-body theorists. More recently, the possibilities for using, and eventually optimizing, these inorganic complexes as circuit elements in spin-dependent electronic transport applications have been entertained both experimentally and computationally.



In this talk, I will provide a brief overview of the experiments that identified the collective phenomena now known as resonant tunneling of magnetization and Berry's phase oscillations and explain why these phenomena are fundamentally and potentially technologically interesting. After doing so, I will discuss the DFT-based (NRLMOL) calculation of electronic structures, magnetic anisotropy Hamiltonians, spin-ordering energies, and Dzyaloshinskii-Moriya interactions in approximately ten molecular magnets that are similar to the $Mn_{12}O_{12}(CH_3COO)_{16}(H_2O)_4$ "type-1 molecular magnet" (aka Mn_{12}). I will discuss why the low-temperature behavior of molecules composed of high-spin metal centers (S >1) may be very accurately described within such spin-unrestricted broken-symmetry single-determinental methods. Conversely, the need for multiconfigurational methods for applications to systems of spin ½ metal centers, such as the $K_6[V_{15}As_6O_{42}(H_2O)]$ "type-2 molecular magnet", and for quantitatively modeling spin-dependent electron transport across all types of molecular magnets be discussed.

The discussion does not necessarily represent the priorities of any government agency.

Host: Professor Connie Lu