

Tuesday Afternoon, November 5, 2002

Molecular and Bio-Magnetism

Room: C-205 - Session MB+BI+OF-TuA

Molecular and Bio-Magnetism

Moderator: M. Grunze, Heidelberg Universität, Germany

2:00pm **MB+BI+OF-TuA1 Single-Molecule Magnets: A Molecular Approach to Nanoscale Magnetic Materials**, **G. Christou**, **M. Soler**, **N. Aliaga-Alcalde**, **S. Bhaduri**, University of Florida, **W. Wernsdorfer**, Laboratoire Louis Neel - CNRS, France, **D.N. Hendrickson**, University of California at San Diego **INVITED**

Single-molecule magnets (SMMs) are molecules that function as single-domain magnetic particles which, below their blocking temperature, exhibit the classical macroscale property of a magnet, namely magnetization hysteresis.¹ SMMs owe their properties to a combination of a large ground state spin value and easy-axis-type anisotropy, which give a significant barrier to magnetization relaxation. SMMs thus represent a molecular (or bottom up) approach to new nanoscale magnetic materials, offering all the advantages of molecular chemistry (room temperature synthesis, purity, solubility in many solvents, a well defined periphery of organic groups, a crystalline ensemble of monodisperse units) as well as displaying the superparamagnetism of a mesoscale magnetic particle. They also display quantum tunneling of magnetization (QTM), emphasizing that they straddle the interface between the classical and quantum regimes. SMMs have many potential applications, but these require that their properties be both understood and controlled, particularly QTM. The Mn₁₂ SMMs are the best understood. Various derivatives have been prepared differing in the organic groups, and it has been discovered that the magnetic properties (including QTM) can be significantly altered. This is also possible by adding additional electrons, and both the [Mn₁₂]⁻ (S = 19/2) and [Mn₁₂]₂⁻ (S = 10) versions have been prepared. Mn₄ SMMs with S = 9/2 have also been extensively studied. In some cases, two Mn₄ SMMs occur as supramolecular dimers, [Mn₄]₂, and exchange interactions between them lead to interesting modifications of their QTM properties, establishing the feasibility of tuning the QTM in SMMs.²

¹ G. Christou, D. Gatteschi, D. N. Hendrickson, and R. Sessoli, MRS Bulletin 25, 66 (2000).

² W. Wernsdorfer, N. Aliaga-Alcalde, D. N. Hendrickson, and G. Christou, Nature 416, 406 (2002).

2:40pm **MB+BI+OF-TuA3 Density-Functional-Based Simulation of Molecular Magnets**, **M.R. Pederson**, **N. Bernstein**, Naval Research Laboratory, **T. Baruah**, Georgetown University, **J. Kortus**, Max-Planck-Institute, Germany **INVITED**

Recently a class of transition-metal containing molecules have attracted significant experimental interest because they retain their magnetic orientation at relatively high temperatures and because they exhibit quantum tunneling of magnetism. These molecular magnets consist of approximately 70-200 atoms and are typically composed of 4-15 transition metal atoms which are held in place by organic ligands and anions. The fundamental figure of merit which governs these phenomena is the magnetic anisotropy which arises due to the spin-orbit interaction and other couplings between spin and spatial degrees of freedom. Recently, a quantum-mechanical method has been developed which allows for the density-functional-based determination of magnetic anisotropies in molecules and clusters.¹ We have used this method to calculate anisotropies in several molecular magnets which include: Mn₁₂O₁₂(RCOO)₁₆(H₂O)₄, Fe₈O₂(OH)₁₂(C₆N₃H₁₅)₆, Co₄C₅NH₄(CH₂O)₄(CH₃OH)₄Cl₄, and [Mn₁₀O₄(2,2'-biphenoxide)₄Br₁₂]⁴⁻. Our calculations show that good agreement between experiment and theory can be obtained. While the reorientation barriers and magnetic resonant tunneling fields are primarily determined from the second-order anisotropy hamiltonian,¹ higher-order effects can change these quantities by about ten percent. Further, such effects determine tunnel splittings and play a significant role in tunneling dynamics. Currently the primary source of such splittings is an active area of investigation. We have recently suggested that vibrationally induced changes in the spin-orbit interaction will contribute to higher-order anisotropies.² Further, computational results on the 4th-order magnetic anisotropy show that this interaction may provide a dominant contribution to the higher-order barriers and that it partially contributes to tunnel splittings. We discuss these calculations and compare our results to the experimental infrared work of Sushkov et al which shows that certain vibrational intensities are strongly perturbed by applied magnetic fields in the Mn₁₂-Acetate system.³ A very brief review of the computational method, NRLMOL, used in this work will be included in the talk.

¹ M.R. Pederson and S.N. Khanna, Phys. Rev. B 60, 9566 (1999).

² M.R. Pederson, N. Bernstein and J. Kortus, (Cond-mate/0201353).

³ A.B. Sushkov, B. Jones, J.L. Musfeldt, et al, Phys. Rev B 65,(2002).

3:20pm **MB+BI+OF-TuA5 Measuring and Manipulating Single Molecules Inside Living Cells**, **J.S. Kanger**, **A.H.B. de Vries**, **J. Greve**, University of Twente, The Netherlands, **B. Krenn**, **R. van Driel**, University of Amsterdam, The Netherlands **INVITED**

For manipulating single molecules, techniques like AFM or optical tweezers are typically used. However, the actual actuators of these systems are relatively large, and therefore we are not able to manipulate single molecules that are situated deep inside the cell (for example inside the nucleus), without causing massive damage to the cell itself. We describe a conceptual simple arrangement for manipulating ultra small magnetic beads inside living cells using magnetic forces. By using magnetic forces to manipulate the bead, and a low yield HeNe laser to measure its position, we are able to generate a relatively high force, without damaging the cell. The setup is designed to measure the movement of a bead with nanometer precision, and apply picoNewton forces on it. Experimental results combined with model calculations show that a force of 15 pN is feasible for a ferrite bead of 50 nm diameter. If a bead is attached to a functioning protein the movement of this protein in the cell can be monitored and manipulated. We plan to apply this technique to the study of chromatin structure function relations inside the living cell. The magnetic force on a bead is proportional to the magnetization of the bead, and the gradient of the magnetic field. To produce a magnetic field that gives a gradient that is controllable both in direction and strength we constructed a four pole configuration. The tips of these poles (5 µm width and height) are placed 20 µm from each other, which leaves enough space to place a cell, with a magnetic bead in the nucleus, between the poles. The magnetic field is guided from external coils to the pole tip that becomes magnetically saturated (1.8 Tesla). The pole tips are produced in the cleanroom facilities of our university. Bead position detection is done by back focal plane interferometry. A low-yield HeNe laser will be focused on the bead. The combination of the laserbeam and, and the forward scattered light gives a interference pattern on a quadrant detector, which is depended on the position of the bead in the focus.

4:00pm **MB+BI+OF-TuA7 Synthesis and Functionalization of Nanoparticles**, **A. Ulman**, Polytechnic University **INVITED**

The talk will focus on metal and metal oxide nanoparticles. A one-phase synthesis of thiolate-functionalized metallic nanoparticles will be described, and further chemical reactions, such as surface-initiated polymerization and attachment of DNA bases will be presented. Sonochemical preparation of oxide and mixed oxide nanoparticles will be reported. We have demonstrated, for the first time, that sonication is a very efficient method for coating of γ-Fe₂O₃ and other oxide nanoparticles. The attachment of enzymes to γ-Fe₂O₃ nanoparticles will be described.

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