Theory and Computation of Molecular Magnetism

Course Overview

Magnetic effects in molecules are ubiquitous in nature and emerge from a combination of spin-orbit coupling, short- and long-range spin-spin interactions, and interactions between external electromagnetic fields, and the spins and charges on the individual particles. At the nanoscale, there are many manifestations of spin-dependent electronic phenomena which can lead to two types of collective behavior in molecular magnets, influence oxygen transport in Heme molecules or chemical reaction rates, mediate photomagnetic behaviors, or simply provide a means for characterization of molecular structure and composition. To understand this wide range of phenomena from a computational and theoretical point of view, density-functional-based electronic-structure methods have proved to be reasonably successful and comparisons between computational predictions and experiment aid in understanding technical gaps that must be addressed to more thoroughly predict spin-dependent properties of molecular-magnetic components. Skills and tools needed for computational understanding of these phenomena can be acquired through applications of electronic structure methods to magnetic molecules that exhibit very well defined single-spin collective behavior.

This proposed mini-course would provide a brief overview of the various behaviors mediated by spin in molecular systems and then focus on the theoretical and computational understanding of such effects from the standpoint of density-functional theory. The course would move from the calculation of the electronic structure of a simple radicals, to single-center magnetic molecules, and then to ligated molecular magnets. Students will learn how to calculate spin-spin exchange coupling parameters and magnetic reorientation barriers (zero-field splittings) in simple molecular magnets and will learn how to determine which type of spin-carrying molecules are likely to exhibit the property of resonant tunneling of magnetization. The latter collective property is of interest to future information technologies and sensing.The final lecture will define existing computational challenges in this field.

Course is designed for advanced undergraduate or graduate/postgraduate researchers. Knowledge of magnetic phenomena at the nanoscale is not required. Students should have knowledge in quantum mechanics and mathematics, and have performed advanced coursework in physical chemistry or physics. Experience with programming and access to a linux-based computer is necessary to perform prototypical calculations.

Dates	**December 15-20, 2016.** **Maximum Number of participants: 60.**
You Can Attend if	Anybody with interest in the course topic and adequate basic training in Physics and Chemistry may attend. Course is designed for advanced undergraduates or graduate/postgraduate researchers. Knowledge of magnetic phenomena at the nanoscale is not required. Students should have knowledge in quantum mechanics and mathematics, and should have performed advanced coursework in physical chemistry or physics. Experience with programming and access to a linux-based computer is necessary to perform prototypical calculations. Selection on the first-come-first-served basis after ensuring reasonable background (total capacity: 60; some seats reserved for students from the Savitribai Phule Pune University). Resume/CV with a brief statement of interest/purpose is required for selection and registration.

Fees	**One-Time GIAN Registration:** Visit http://www.gian.iitkgp.ac.in/GREGN/ **Course Fees:** Those affiliated to Savitribai Phule Pune University or affiliated colleges: No fee, but registration is must. Those affiliated to academic institutions, research institutes, NGOs, etc.: ₹1000. Those from industry: ₹5000. Those from abroad: US $ 150. Fees include tea with light snacks, any instructional material provided by the expert faculty, computer access during any tutorial sessions for the course, internet access via the SPPU campus network during the course. Out-station candidates need to arrange for transport and accommodation on their own. Minimum 90% attendance necessary to be eligible for certificate of participation/attendance. Appearing for evaluations/examinations during the course is necessary for certificate of grades in the course.

Mark R Pederson is a Research Professor at Johns Hopkins University in the Department of Chemistry since 2013. After receiving his PhD in Theoretical Physics at the University of Wisconsin-Madison (1986), Pederson moved to the Naval Research Laboratory and served first as a postdoctoral researcher, then as a single-investigator, and eventually as the head of the “Theory of Molecules and Nanoscale Devices” section within the Center for Computational Materials Science at the Naval Research Laboratory. Pederson is the lead developer of a computational density-functional-based electronic structure code for molecules and clusters (NRLMOL). Pederson’s research has concentrated on the development, testing, and application of this massively parallel electronic structure method for calculations of electronic structure, vibrational spectroscopy, chemical-vapor deposition, fullerenes, molecular magnetism, and organic photovoltaics. Pederson is a fellow of the American Physical Society and a member of the American Chemical Society and the Materials Research Society. Dr. Pederson has coauthored over 210 papers in areas related to density-functional-based design and simulation of molecular and material systems and is recognized as a pioneer in the area of density-functional-based understanding of molecular magnetism.

Course Coordinator

Anjali Kshirsagar

V L Mathe

Department of Physics

Savitribai Phule Pune University

Pune 411007

Phone: 20-25692678, 20-25601408,ext 200 or 331 on both lines, 20-25694224

Email: gian@physics.unipune.ac.in

Web: http://physics.unipune.ac.in/

GIAN One-Time Registration

http://www.gian.iitkgp.ac.in/GREGN/