Dept. of Physics & Engineering Physics
Fall 2021 Physics Colloquium Series

remotely via ZOOM
Monday, September 13, 03:00-04:30 pm

Undergraduate and Graduate Research in Physics: Vexing Challenges for Today, Opportunities for Tomorrow

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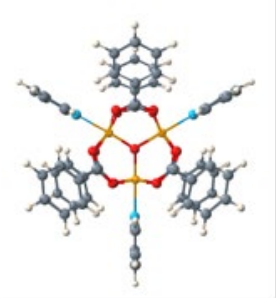
Before discussing molecular magnets and their current importance to quantum science, I will describe my adventures in science that began with the University of Michigan Proton Decay Experiment as an undergraduate and a circular path from a fundamental problem in density functional theory as a graduate student to molecular magnets and back again to self-interaction corrected density functional theory. I will discuss why hard working undergraduate and graduate students in physics continue to have a wide range of promising career choices and why society continues to rely upon physical scientists to address the challenges of the day.



The size range and deceptive complexity albeit behavioral simplicity of molecular magnets attracts physical scientists from many disciplines and challenges them to understand how 50-100 nuclei and 200-1000 electrons can exhibit such simple collective behavior. For example, quantum tunneling of magnetization, which occurs in broken-spin-symmetry magnetic molecules illustrates the power of density-functional-based pictures for predicting both the magnetic strength of molecules and the magnetic fields at which quantum tunneling occurs. Alternatively, the spin-electric effect explicitly challenges the notion that single-determinantal theories can describe the physics leading this phenomenon. However, the large molecular size resists quantitative quantum chemical explanations and a combination of model Hamiltonians with density-functional treatments are the optimal means for exploring these intrinsically multi-configurational problems. I will review previous work on the Cu_3 molecular magnet and show how the combination of broken symmetry density-functional theory, with simple self-interaction corrections and spin-orbit inclusion, can be used to derive three-spin Heisenberg Hamiltonians that describe the Dzyaloshinskii-Moriya induced splitting of degenerate low-energy Kramer doublets into S=1/2 chiral and anti-chiral pairs. The resulting energy level diagrams will be compared to that of a three-quark system.

The second half of this talk features the $Fe_3O(NC5H5)_3(O2CC6H5)_6$ molecule that is the first possible spin-electric system based upon spin 5/2.centers. As a curiosity, I discuss the rather unusual point-group symmetry, which includes a rotation matrix appearing in elementary particle wavefunctions, that we call Rq. Using standard density-functional methods we show that the spin-electric behavior of this molecule could be more interesting due to energetically competitive reference states with high and low local spins (S=5/2 vs. S=1/2) on the Fe^{3+} ions. We provide spectroscopies to deduce the presence of both states and note that similar multiferroic behavior exists in the Mn_3 molecular magnet. Rationale for use of a new version to self-interaction corrections, FLOSIC, to improve quantitative predictions, especially in lanthanide systems, will be included.

$$R_Q \equiv \begin{pmatrix} \frac{1}{3} & -\frac{2}{3} & -\frac{2}{3} \\ -\frac{2}{3} & \frac{1}{3} & -\frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{1}{3} \end{pmatrix}$$

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Mark R. Pederson

- BS Physics University of Michigan – Worked on Proton Decay experiments (Larry Sulak and Rick Bionta) and Open Resonators (Professor Bill Williams and Carl Weiman)
- PhD Physics University of Wisconsin (Professor Chun Lin) – Dissertation: Self Interaction Corrections to Density Functional Theory
- Postdoc (Professor Barry M Klein)
- Research Scientist and Supervisory Research Physicist NRL – 20 years
- Sabbaticals at Max-Planck Institute – Stuttgart and National Science Foundation
- Eleven years as program manager in Computational and Theoretical Chemistry – Department of Energy
- Professor and Chair – Department of Physics, University of Texas El Paso
- Also hold the Dr. C. Sharp Cook Endowed Chair in Physics at UTEP

Developed NRLMOL – First massively parallel electronic structure code for molecules. Developed new Fermi-Lowdin-Orbital self-interaction corrections in 2014

Past interests: Fullerenes, Diamond Grown, Defects in Diamond, Molecular Magnets, IR/Raman Spectroscopy (all computational)

Current interests: Molecular Magnetism, Quantum Sensing, Quantum Information, Quantum Emulators, Spin Hamiltonians, Computational Materials and Chemical Sciences

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Dr. Pederson holds the C. Sharp Cooke Chair in Physics at the University of Texas at El Paso.
His research background is in chemical physics, condensed-matter physics, and computational physics. He received his doctoral degree from the University of Wisconsin-Madison – where he was recognized as a Distinguished Alumni in the Department of Physics – and bachelor's degree from the University of Michigan, Ann Arbor. Dr. Pederson spent his career performing, managing, and funding research at the interface of physics and chemistry for the Naval Research Laboratory (NRL) in Washington, D.C., the National Science Foundation, and most recently for the DOE. Since the start of his career, Dr. Pederson's focus has continuously concentrated on next-generation computing paradigms for quantum mechanics. Dr. Pederson is the primary author of the Naval Research Laboratory Molecular Orbital Library (NRLMOL), a code that is used to benchmark several versions of the density functional theory for molecules. It is the first computational code capable of calculating infrared and Raman spectra of molecules within density functional theory, and the first code to calculate several types of magnetic responses of molecules to applied magnetic fields.

In 2014, Dr. Pederson invented a new form of density-functional theory that he named the "Fermi-Löwdin-Orbital Self-Interaction Correction".

Dr. Pederson enjoys travel, the outdoors, endurance sports, and adventure. He enjoys running and biking, and has completed four marathons. He has swam across the Chesapeake Bay, camped in the frozen Minnesota Boundary waters in the middle of the winter, and bicycled from Munich to Budapest.