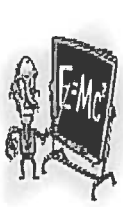

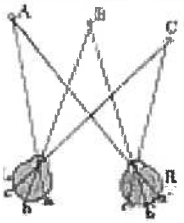

WEEKLY CALENDAR

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March 19, 2007

Special Seminar

" THEORETICAL APPROACH TO AB-INITIO CALCULATIONS OF NMR SPECTRA FOR LARGE BIO-MOLECULES"

3:40PM / Monday, 19 March 2007 / Room 109

[Refreshments served at 3:15 PM in Room 229 Nicholson]

Host: Dr. John DiTusa

Timo Thonhauser, Ph.D.
MIT and Rutgers University

Magnetization is a fundamental concept that we teach all undergraduates. Thus, it is truly extraordinary that there was, until our recent work, no generally accepted formula for the orbital magnetization of a periodic solid. In this talk, I present a Wannier-function approach that allows us to solve this long-standing problem and derive an analytic quantum-mechanical expression for the orbital magnetization in extended systems [Phys. Rev. Lett. 95, 137205 (2005)]. I will then outline a novel way to calculate NMR shielding tensors completely based on our theory of orbital magnetization. The NMR shielding is of particular interest in large biological systems, many of which have significant van der Waals interactions. Effective calculations for these systems become possible due to our recently developed DFT exchange-correlation functional that includes van der Waals interactions in a seamless manner. Tantalizing future applications are studies of large biological systems such as the oligomeric protein aggregates that are toxic in neurological disorders like Alzheimer's and Parkinson's diseases.

Special Seminar

"Radioactive Nuclei in the Cosmos"

3:40PM / Thursday, 22 March 2007 / Room 109

[Refreshments served at 3:15 PM in Room 229 Nicholson]

Host: Dr. Jerry Draayer

Jeff Blackmon, Ph.D.
Oak Ridge National Laboratory

Radioactive atomic nuclei play an important role in many astrophysical environments, particularly in stellar explosions. The decay of radioactive nuclei and nuclear reactions involving radioactive nuclei are an important source of energy generation in novae and X-ray bursts, the most common stellar explosions in our Galaxy. Many of the heavy elements are synthesized in supernovae via neutron capture on short-lived neutron-rich nuclei. New observations are helping to improve our understanding of stellar explosions and the origins of the heavy elements, but our understanding is hindered by the limited nuclear data available on unstable nuclei. The study of short-lived nuclei is now a major focus of many laboratories including two national user facilities, the Holifield Radioactive Ion Beam Facility (HRIBF) at Oak Ridge National Laboratory and the National Superconducting Cyclotron Laboratory (NSCL) at Michigan State University. Construction of an advanced radioactive ion beam facility is also planned by the U.S. Department of Energy during the next decade. I will review some of the recent experimental work with radioactive ion beams that is helping to improve our understanding of stellar explosions. I will summarize the current state of our knowledge and provide an outlook for the future.

(continued)

Material Science and Engineering Seminar

"Superconductivity in Non-centrosymmetric Materials"

3:40PM / Tuesday, 21 March 2007 / Room 109

Host: Dr. Ilya Vekhter

Daniel Agterberg, Ph.D.
University of Wisconsin-Milwaukee

The absence of inversion symmetry has a pronounced effect on the quasi-particle states through the splitting of the usually spin degenerate bands. This in turn influences the superconducting state, which relies on quasi-particle degeneracy under time reversal and parity symmetries to form Cooper pairs. It is relatively easy to remove time-reversal symmetry (with magnetic fields for example) but manipulating parity symmetry in superconductors is not straightforward. Superconductivity in non-centrosymmetric materials therefore provides a unique opportunity in this respect. Theoretical results on non-centrosymmetric superconductors will be presented with an emphasis on the recently discovered materials CePt3Si, CeRhSi3, CeIrSi3, KOs2O6, and Li2Pt3B. This will include discussion of the appearance of lines nodes in the energy gap due to the mixing of spin-singlet and spin-triplet order parameters; the spin susceptibility for predominantly spin-singlet or spin-triplet pairing; and new physics that appears due to the application of magnetic fields in these superconductors.

Special Seminar

"Probing the Limits of Nuclear Existence through Decay Spectroscopy"

3:40PM / Monday, 26 March 2007 / Room 109

[Refreshments served at 3:15 PM in Room 229 Nicholson]

Host: Dr. Jerry Draayer

Sean Liddick, Ph.D.
University of Tennessee

The limits of nuclear stability is a fundamental question in nuclear physics. The location of the driplines (defined as when an additional nucleon is no longer bound to the nucleus) is theoretically difficult predict and requires significant experimental input. Predicting the limits is complicated by the fact that nuclear structure is a dynamic characteristic and can change as one moves away from the valley of stability. Both the limits of nuclear existence and the dynamic nature of nuclear structure also affect the astrophysical processes responsible for the creation of the elements. Decay spectroscopy has become a valuable tool for measuring nuclear properties at low counts rates in an effort to learn about the nuclear structure and the limits of stability. Recent results on particle (alpha and proton) decaying nuclei will be given along with the implications for nuclear structure and astrophysics. These results will include the discovery of two new isotopes (109Xe and 105Te),a sensitive measurement of alpha decay in 109I and its affect on the astrophysical rp-process, and the first digital pictures of a nuclear decay (2 proton decay in this case) from 45Fe.