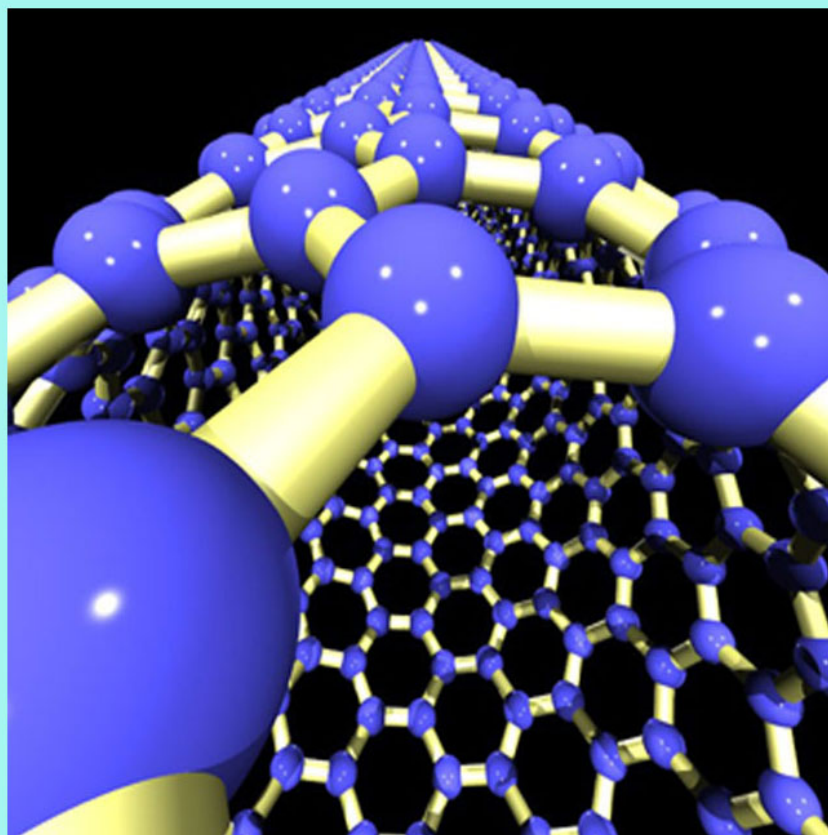


# 2006 FRONTIERS IN CHEMICAL PHYSICS WORKSHOP



Research the Interface Between Chemistry & Physics

- > Nanoscience
- > Multifunctionality
- > Chirality
- > Molecular Magnets
- > Electronic Structure Theory
- > and MORE !

16th - 18th  
February, 2006



Sponsored by the Presidents Innovation Fund for Teaching, Research & Services at UT  
Organized by the Chemical Physics Program, University of Tennessee

## **2006 Frontiers in Chemical Physics Workshop University of Tennessee**

Each spring, we host a workshop to highlight important areas in Chemical Physics. The three day event consists of presentations by internationally acclaimed speakers, a graduate student round table discussion, an informal "Saturday Session" that includes local ORNL, UT, and visiting speakers, plenty of time for discussion, and a reception. The Frontiers in Chemical Physics Workshop is an important part of the dynamic scientific environment for interdisciplinary research at the University of Tennessee.

Chemical Physics is an exciting and interdisciplinary area of science lying midway between the traditional fields of Chemistry and Physics. Although interdisciplinary in character, the field of Chemical Physics is quite broad, covering everything from elementary excitations in atoms, to the theory of weakly bond complexes, to nanoscience and technology involving novel materials. Chemical Physicists tend to focus on solving complex problems, using a variety of experimental and theoretical techniques from different areas of science to understand the fundamental properties of nature.

### Useful phone numbers

Cumberland House Hotel	865-971-4663
Department of Chemistry	865-974-3141
Janice L. Musfeldt	865-974-3392
Robert Compton	865-974-1069

**Wish you a pleasant and fruitful workshop.**

**Janice L. Musfeldt  
Robert Compton**

**SCHEDULE**  
**2006 Frontiers in Chemical Physics Workshop**  
**University of Tennessee**

**Thursday, February 16, 2006**

12:30 pm Lunch at University Club

2:00 pm Graduate Students: Round Table Discussion  
Location: 511 Buehler Hall, University of Tennessee

3:30 pm **Gabor Somorjai**                      The Nanoscience Revolution: The  
Berkeley                                      Merging of Colloid Science, Catalysis  
and Nanoelectronics  
Location: SERF 307

6:00 pm Dinner  
James White's Fort in Knoxville

## Friday, February 17, 2006

All presentations are in SERF 307, University of Tennessee

- |          |   |  |
|----------|---|--|
| 9:00 am  | <b>Jack Simons</b><br>Utah  | How Very Low-Energy Electrons Break Strong Bonds in DNA and Peptides                                       |
| 10:00 am | <b>James Coe</b><br>Ohio State  | Surface-Plasmon-Mediated Extraordinary Infrared Transmission of Metal Arrays with Subwavelength Holes      |
| 11:00 pm | <b>Peer Fischer</b><br>Harvard  | New Forms of Chiral Spectroscopy   |
| 12:00 pm | Lunch Break & Coffee  |  |
| 1:00 pm  | <b>Gotthard Seifert</b><br>Dresden  | Inorganic Nanotubes, Fullerenes and Platelets – Structure, Stability, Electronic and Mechanical Properties |
| 2:00 pm  | <b>Sang-Wook Chenog</b><br>Rutgers  | Multifunctional Multiferroics  |
| 3:00 pm  | <b>Marshall Luban</b><br>Ames Lab   | Interdisciplniary Adventures in Magnetic Molecules – Why YOU Should Enlist, Now!                           |
| 4:00 pm  | Lab Tours and Discussions   |  |
| 6:00 pm  | <b>Dinner and Reception,<br/>Downtown Gallery and Emporium<br/>All are welcome!</b> |  |

## Saturday, February 18, 2006

All presentations are in SERF 307, University of Tennessee

- |          |   |  |
|----------|---|--|
| 9:30 am  | <b>Bruse Bursten</b><br>University of Tennessee       | Electronic Structure of Novel Actinides  |
| 10:15 am | <b>Khaled Al-Hassanieh</b><br>University of Tennessee | Electron Transport in Quantum Dots and Molecular Conductors  |
| 11:00 am | <b>David Schultz</b><br>Oak Ridge National Laboratory | Astrophysical Puzzles and Chemical Physics Clues: Unraveling the Message of the H <sub>2</sub> Spectrum within the Interstellar Medium |
| 12:00 pm | Box Lunches – Panera’s                                |  |
| 1:00 pm  | <b>Jian Shen</b><br>Oak Ridge National Laboratory     | Taming Electronic Spins in Conjugated Polymers   |
| 1:45 pm  | <b>Jason Haraldsen</b><br>University of Tennessee     | Properties of the Smallest Molecular Magnets   |
| 2:30 pm  | <b>Vince Meunier</b><br>Oak Ridge National Laboratory | Molecular Nanoelectronics: Simulating and Designing Devices on the Nanoscale   |

*2006 Frontiers in  
Chemical Physics Workshop*

**Thursday, Feb 16<sup>th</sup> to Saturday, Feb 18<sup>th</sup> 2006  
University of Tennessee, Knoxville**

**ABSTRACTS**

## **The Nanoscience Revolution: The Merging of Colloid Science, Catalysis and Nanoelectronics**

**Gabor A. Somorjai, Department of Chemistry and Lawrence Berkeley National Laboratory, University of California, Berkeley**

Size reduction of active structures utilized in surface technologies approaches the nanometer regime. The electronic and atomic structural properties of semiconductors and metals change dramatically on the nanoscale. Monodispersed nanoparticles can be fabricated either by size reduction lithography or can be grown in solution capped by surfactants or polymers using colloid science methods. Metal catalysts are nanoparticles deposited on oxide surfaces in 2-dimensional or 3-dimensional configurations. Nanoscience provides opportunities to develop catalytic processes with enzyme-like 100% selectivity toward desired products (green chemistry) and to develop new ways of energy conversion. Catalytic reaction studies revealed that oxide-metal interfaces are active sites for many reactions. There is evidence for continuous flow of hot electrons during exothermic catalytic reactions across the oxide-metal interface that behaves as a Schottky diode. Nano-bioengineering benefits from using nanopatterned polymer surfaces and determination of the structures of polypeptides adsorbed on hydrophilic and hydrophobic surfaces.

## **How Very Low-Energy Electrons Break Strong Bonds in DNA and Peptides**

**Jack Simons, University of Utah**

Recent experimental and theoretical work has shown that very low-energy electrons (e.g., 0-3 eV) can attach to DNA and induce strand breaks. Where the electron likely attaches, what bond(s) breaks, and how this happens have been the subject of much of our group's efforts, and this presentation will summarize our findings to date. In addition, low-energy electrons are used in mass spectrometry to induce very characteristic backbone bond cleavages in positively charged peptide and protein samples. Again, the issues are where the electrons attach, what bonds are cleaved, and how this occurs. This presentation will detail our efforts to address these questions including our suggestion that nearby positive sites can stabilize anti-bonding orbitals via Coulomb stabilization. Most, if not all, of the electron-attached species examined here are electronically metastable, so special theoretical methods must be used to handle them.

## **Surface-Plasmon-Mediated Extraordinary Infrared Transmission of Metal Arrays with Subwavelength Holes**

**James Coe, Ohio State University**

Optically thick metal films with patterns of subwavelength holes have been shown to transmit more light than is incident on the holes alone, i.e. they exhibit Ebbesen's extraordinary transmission effect. We have moved this effect into the infrared region and observed more than 100-fold enhancements over literature reports in vibrational absorption spectra of molecules at the surface of the metal. Basic optical physics of the surface-plasmon-mediated transmission resonances will be explored and then applications will be discussed, such as enhanced absorption spectroscopy, control of the flow of light through microchannels, and stacked-mesh sensors.

## New Forms of Chiral Spectroscopy

**Peer Fischer, Harvard University**

The fundamental importance of chirality in chemistry and biology requires analytical probes that are sensitive enough to distinguish between the two mirror-image forms (enantiomers) of a chiral molecule. The enantiomers of a chiral molecule are, despite clear differences in biological action, exactly alike in all chemical and physical properties except those that involve a left-right difference. This makes the detection, discrimination and study of chiral molecules especially challenging. Only under a chiral influence, such as another chiral molecule or circularly polarized light, can interactions distinguish between the two enantiomers of a chiral molecule. We discuss how linear optics, nonlinear optics, and NMR can be sensitive to chirality.

Optical activity in linear optics is briefly reviewed and the symmetry requirements of a chiral observable are discussed. An alternative approach to optical rotatory dispersion (ORD) measurements is presented, which is based on an effect that Fresnel proposed in 1822 and that we have recently observed. It is then shown that chiral observables in nonlinear optics can be described by selection rules that entail new physics and do not necessarily require the use of circularly polarized light to detect chirality. Examples are presented from our work on sum-frequency generation in liquids. Finally, we discuss how chirality may be directly detected in liquid-state NMR spectroscopy without the presence of a chiral reagent or solvent -- even though the chemical shifts and spin-spin coupling are identical for the two enantiomers.

## **Inorganic Nanotubes, Fullerenes and Platelets - Structure, Stability, Electronic and Mechanical Properties**

**Gotthard Seifert, Technische Universitat Dresden**

Since the discovery of carbon nanotubes and fullerenes, tubular and fullerene-like structures have become a challenging new field of research in solid state physics, chemistry and materials science. Therefore, theoretical investigations for understanding of their structures, properties and formation mechanism are very important. Of special interest is the transition to a quasi one dimensional system, as it has been realized in tubular structures (nanotubes) from carbon, metal chalcogenides and other materials. The stability and the possible existence of non-carbon nanotubes, their electronic structure, their stability and their mechanical properties are discussed on the basis of general arguments by a conformal mapping of two-dimensional layer structures onto the surface of a cylinder and by Density-Functional-Theory based calculations. The stability of fullerene like cage structures is viewed critically. Furthermore, the specific properties of two dimensional, platelet like structures will be discussed also.

## **Multifunctional Multiferroics**

**Sang-Wook Cheong, Rutgers Center for Emergent Materials**

Ferroelectric and magnetic materials have been a time-honored subject of study and have led to some of the most important technological advances to date. Magnetism and ferroelectricity are involved with local unpaired spins and local dipoles (originating from off-center structural distortions), respectively. These two seemingly unrelated phenomena can coexist in certain unusual materials, termed multiferroics. Despite the possible coexistence of ferroelectricity and magnetism, a pronounced interplay between these properties has rarely been observed. This has prevented the realization of multiferroic devices offering such functionality. We will discuss newly-discovered, extraordinary coupling between spin and lattice degrees of freedom in a certain class of multiferroics. For example, the highly reproducible electric polarization reversal in  $\text{TbMn}_2\text{O}_5$  and  $\text{TbMnO}_3$  and unprecedented large change of dielectric constant in  $\text{DyMn}_2\text{O}_5$  and  $\text{DyMnO}_3$  can be activated by an applied magnetic field ( $H$ ). In addition, acoustic phonons in hexagonal- $\text{HoMnO}_3$  can be significantly influenced by  $H$ . These manifestations of giant spin/lattice coupling provide new device concepts with tunable multifunctionality.

## **Interdisciplinary Adventures in Magnetic Molecules – Why YOU Should Enlist, Now!**

**Marshall Luban, Ames Laboratory (USDOE) and Iowa State University**

Crystalline samples of magnetic molecules provide a new and rich platform for exploring fundamental issues in nanomagnetism as well as for potential applications. The most critical players are the synthetic chemists who are creating new, sometimes astounding, systems at a very rapid pace. As a result of strong collaborative efforts by chemists and physicists, employing a large arsenal of experimental and theoretical tools, significant progress is being made towards understanding some of the major phenomena. Thermodynamic measurements, pulsed magnetic field studies, inelastic neutron scattering, and optical and resonance techniques are some of the effective experimental tools in use. Comparison with experiment can in many cases be made by employing a toolbox that includes the quantum Monte Carlo method for low-spin ions, the classical Monte Carlo method for high-spin ions, effective matrix diagonalization methods, and approximate statistical mechanical methods based on solvable classical and quantum models. The novel feature of magnetic molecules is that the magnetic properties of crystalline samples are almost exclusively determined by Heisenberg exchange interactions between the magnetic ions embedded in the individual molecules, while intermolecular magnetic interactions can usually be ignored. I will provide an introduction that highlights examples of known magnetic molecules and the major issues which these spawn. Also, for several rather complex magnetic molecules, I will give some recent theoretical results that are in good agreement with experiment. One major message of this talk is that this field is young enough so that you can still acquire a large and comfortable acreage.

**Electronic Structure of Novel Actinides**

**Bruce Bursten, University of Tennessee**

TBA

## **Electron Transport in Quantum Dots and Molecular Conductors**

**Khaled A. Al-Hassanieh, University of Tennessee**

Electron transport in nanostructures such as quantum dots (QD's) and molecular conductors (MC's) has received a great deal of attention in the past decade. These systems are crucial for novel potential applications such as quantum computing and molecular electronics. Due to their small sizes and confined structure, the energy levels in QD's and MC's are quantized, and the electron-electron correlations are dominant, thus leading to interesting effects such as Coulomb blockade and Kondo effect. In addition, other effects such as the phase coherence and electron-phonon interactions play an important role and have been observed in several experiments. I will present a general overview of nanotransport, showing both experimental results and theoretical models. Then I will present a summary of the results of our numerical studies, focusing on electron-phonon interaction and interference effects.

## **Astrophysical Puzzles and Chemical Physics Clues: Unraveling the Message of the H<sub>2</sub> Spectrum within the Interstellar Medium**

**David Schultz, Oak Ridge National Laboratory**

Molecular hydrogen is the most abundant chemical species in the Universe and therefore plays a significant role in astrophysical environments such as starburst galaxies, interstellar molecular clouds, and star-forming regions. However, the scarcity of both accurate and complete data sets for rovibrational inelastic cross sections involving collisions with H<sub>2</sub> has set a serious limitation on the development of reliable astrophysical models. In particular, the investigation of cooling processes, molecular emission, and non-equilibrium effects in molecular gaseous nebulae and other molecular environments requires collisional excitation data for H-, He-, and H<sub>2</sub>-impact on H<sub>2</sub>. Recently, a number of observations, performed using the NASA Spitzer Space Telescope's infrared spectrograph, have identified emissions arising from pure rotational transitions in H<sub>2</sub>. To interpret these spectral lines, an accurate set of data for thousands of cross sections is needed, thus requiring large scale molecular physics computer codes to make extensive theoretical predictions.

## **Taming Electronic Spins in Conjugated Polymers**

**Jian Shen, Oak Ridge National Laboratory**

Conjugated polymers are introducing a new dimension for technological applications including solar cells, large-area flexible solid-state lighting, and lasers. The grand challenge is to tailor the formation and dissociation of singlet and triplet excitons in order to maximize the efficiency of photovoltaic response and electroluminescence (EL). We used a radically new approach to meet the challenge, namely introducing and controlling the electronic spin degree of freedom in the polymers. Specifically, we have doped the polymers with magnetic nanowires, and use spin injection and spin-polarized charge transfer to control the singlet and triplet exciton density in conjugated polymers. Our results indicate that doping of magnetic nanowires can significantly enhance the photocurrent and the EL efficiency of the polymers.

## **Properties of the Smallest Molecular Magnets**

**Jason Haraldsen**

The smallest known nano-scale molecular magnets are materials that contain isolated spin clusters of just a few magnetic ions. The magnetism in these materials can often be described by the nearest-neighbor spin-spin Heisenberg Hamiltonian. Assuming this model we can calculate various observables, including bulk magnetic properties and neutron scattering response functions. We present some applications of these results to real dimer, trimer and tetramer systems.

## **Molecular Nanoelectronics : Simulating and Designing Devices on the Nanoscale**

**Vincent Meunier, Oak Ridge National Laboratory**

The combination of state-of-the-art quantum chemistry methods, efficient numerical algorithms, and high performance computing allows for realistic evaluation of properties at length scales that are routinely reached experimentally. We have coupled large-scale quantum electronic structure calculations with non-equilibrium Green function formulation for determining the quantum conductance on a number of molecular systems. Two illustrations of our method are presented. First, quantum chemical calculations using up to 10,000 localized basis functions are used to investigate electronic properties of doped carbon nanotubes by encapsulation of organic molecules [J. Chem. Phys. 123, 024705 (2005)]. In a second example, we investigated the electron transport properties of a Si/organic-molecule/Si junction using a numerically optimized basis [Phys. Rev. Lett. 95, 206805 (2005)] In both cases, the efficiency of the numerical approach permits the inclusion of a large number of atoms and in turn allows for a realistic description of electronic processes governing transport at the nanoscale.

Speakers List  
2006 Frontiers in  
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University of Tennessee, Knoxville

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