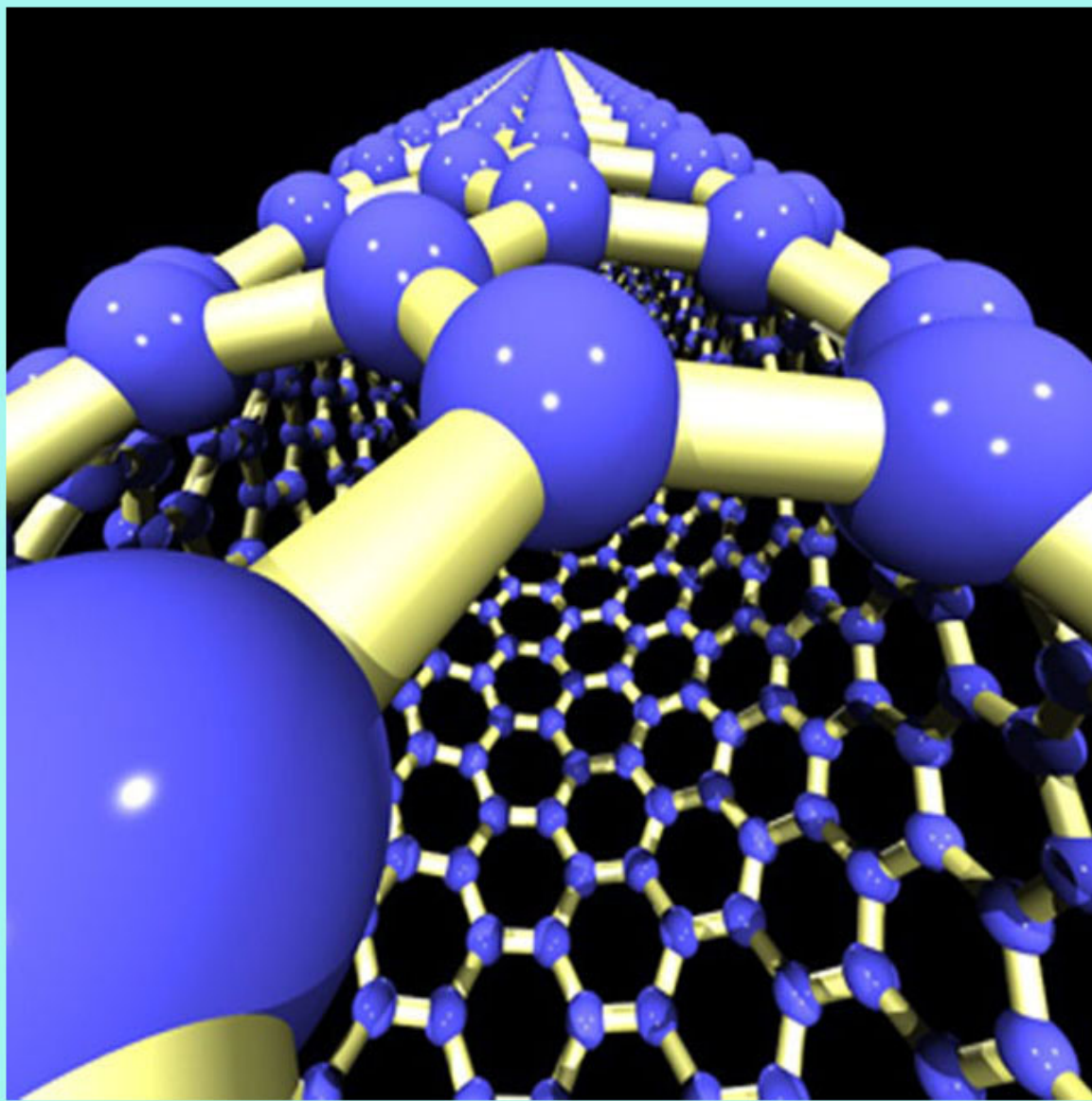


2005 FRONTIERS IN CHEMICAL PHYSICS WORKSHOP



Research the Interface Between Chemistry & Physics

- > Photo & Radiation Physics of Biomaterials
- > Nanocarbon Science
- > Surface Interactions
- > and MORE !

10th - 12th
February, 2005



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

2005 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

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Downtown Radisson	865-522-2600
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
2005 Frontiers in Chemical Physics Workshop
University of Tennessee

Thursday, February 10, 2005

- 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 **R. James Cross Jr.** Finding Fulfillment in the Filling of
Yale University Fullerenes
Location: 415 Buehler Hall, University of Tennessee
- 6:00 pm Dinner & Reception
McClung Museum, UT Campus

Friday, February 11, 2005

All presentations are in Room 511 Buehler Hall, Department of Chemistry
University of Tennessee

- 9:00 am **Leon Sanche** Mechanisms of DNA Damage Induced by
Université de Sherbrooke Low Energy Electrons
- 10:00 am **Sara Majetich** Magnetic Properties of Self-Assembled
Carnegie Melon University Nanoparticle Assemblies
- 11:00 pm **Satish Kumar** Polymer/Carbon Nanotube Composites :
Georgia Institute of Tech. Challenges and Opportunities
- 12:00 pm Lunch Break
- 1:00 pm **Matthew Platz** Time Resolved Spectroscopy of Nitrenes
Ohio State University and Nitrenoids in Solution
- 2:00 pm **Sumit Mazumdar** Universal Features of Quasi-One-
University of Arizona Dimensional Excitons in Pi-Conjugated
Polymers and Semiconducting Single-
Walled Carbon Nanotubes

Friday, February 11, 2005

- 3:00 pm **Rigberto Hernandez** Patterning a Layer by Tickling the Surface
Georgia Institute of Tech
- 4:00 pm Lab Tours
- 6:00 pm Lunch @ Regas Restaurant

Saturday, February 12, 2005

All presentations are in Room 511 Buehler Hall, Department of Chemistry
University of Tennessee

- 9:00 am Coffee & Bagels - Panera's
- 9:30 am **Elias Greenbaum** Nanoscale Photosynthesis, Molecular
Oak Ridge National Interactions, and the Photocatalytic
Laboratory Evolution of Hydrogen
- 10:15 am **David Ball** Single-Molecule Detection and Imaging
University of Tennessee
Space Institute
- 11:00 am **Doug Lowndes** Chemical Physics on the Nanoscience
University of Tennessee & Frontier: Update on the CNMS and
Oak Ridge National Research Highlights in Functional Carbon-
Laboratory Based Nanomaterials
- 11:45 am **A.C. Buchanan III** Organic Radical Reactions in Mesoporous
Oak Ridge National Silica: Impact of Pore Surface
Laboratory Confinement
- 12:30 pm Box Lunches – Panera's
- 1:30 pm **Gerard M. Ludtka** Exploring Ultrahigh Magnetic Field
Oak Ridge National Processing of Materials for Developing
Laboratory Customized Microstructures and Enhanced
Performance
- 2:15 pm **Jeffrey Steill** FT-IR of Trace Gases: Atmospheric
University of Tennessee Analysis and Ionization Products
- 3:00 pm **Thomas Schulthess** Electronic Structure of Dilute Magnetic
Oak Ridge National Semiconductors: A Comparison of the
Laboratory SIC-LSD and the LDA+U methods

***2005 Frontiers in
Chemical Physics Workshop***

**Thursday, Feb 10th to Saturday, Feb 12th 2005
University of Tennessee, Knoxville**

ABSTRACTS

Finding Fulfillment in the Filling of Fullerenes

R. James Cross, Jr., Yale University

We have devised several ways to put noble gas atoms and small molecules inside fullerenes, where they remain trapped. These are stable, van der Waals molecules, since there is no chemical bond to the fullerene. The noble gas atom can serve as an inert label in chemical reactions. ^3He NMR of ^3He -labeled fullerenes and their derivatives is a sensitive probe of the electronic structure of the fullerene and is a useful way to follow a chemical reaction. We have studied the escape of noble gas atoms from fullerenes with chemically opened holes in them.

Mechanisms of DNA Damage Induced by Low Energy Electrons

Léon Sanche, Université de Sherbrooke

Low-energy electrons (LEEs) are produced in large quantities in any type of material irradiated by high-energy particles. In biological media, these electrons can fragment molecules and lead to the formation of highly reactive radicals and ions. Within biological cells, both LEEs and the species they generate can damage DNA, which may lead to mutations or cell death. To investigate, both theoretically and experimentally, the action of LEEs on DNA it is necessary, not only to perform calculations and experiments on the entire molecule, but also on model biomolecular systems. These latter can be made of a basic subunit of the molecule, or a longer portion of it, immersed in different environments to mimic specific cellular conditions. The target molecules usually consist of a multilayer film deposited on a metal substrate bombarded by a LEE beam (0-45 eV) under ultra high vacuum (UHV) conditions. Depending on the experiment, it is possible to measure neutral fragments or ions emanating from these films. The products remaining in the films can be analyzed in situ by X-ray photoelectron and electron energy loss spectroscopies; they can also be removed from the UHV system and analyzed by HPLC and GC/MS. At the theoretical level, it is possible to treat electron attachment to and dissociation from the entire DNA molecule with our newly developed framework or from segments of DNA using Density Functional Theory. By comparing the results of the theory and different experiments, it is possible to determine fundamental mechanisms, operative within DNA, that are involved in the dissociation of basic DNA constituents and the production of single- and double-strand breaks. Such mechanisms involve

- (1) the formation of transient anions which play a dominant role in the fragmentation of all biomolecules investigated
- (2) dipolar dissociation which produces an anion and cation and
- (3) reactive scattering which induces non-thermal reactions.

The transient anions fragment molecules by decaying into dissociative electronically excited states or by dissociating into a stable anion and a neutral radical. These fragments usually initiate other reactions with nearby molecules, causing further chemical damage. The damage caused by transient anions is dependent on the molecular environment. Thus, it appears that changes in the environment or topology of DNA may affect considerably the damage induced by LEEs and may therefore serve as a tool to modify DNA damage induced by high-energy radiation. The results of recent experiments performed on films of DNA and its basic subunits (i.e., H₂O, DNA bases and sugar analogs) and amino acids will be presented at this conference. The major type of experiments will be briefly described and the results of theoretical studies summarized. Application of some of our results to

radiotherapy will be discussed in the context multidisciplinary research. Some of the challenges lying ahead will also be mentioned. This research is financed by the Canadian Institutes of Health Research and the National Cancer Institute of Canada.

- . For a review see L. Sanche, *Mass Spectr. Rev.* 21, 349 (2002).
- . L.G. Caron and L. Sanche, *Phys. Rev. Lett.* 91, 113201-1 (2003).
- . X. Li, M.D. Sevilla and L. Sanche, *JACS* 125, 13668 (2003)

Magnetic Properties of Self-Assembled Nanoparticle Assemblies

Sara Majetich, Dorothy F. Farrell, Yi Ding, Yuhang Cheng,
Carnegie Mellon University

We describe the preparation and properties of highly monodisperse iron, cobalt, and iron platinum nanoparticles, and nanostructures made from them. All of the surfactant-coated nanoparticles are prepared by high temperature solution chemistry methods. We examine two case studies that illustrate the potential of these particles for improving our understanding of nanomagnetism.

In the first, the magnetostatic interactions among monodisperse Fe nanoparticles are varied by changing the particle size, spacing, and degree of structural ordering. The length scale structural order is quantified by small angle x-ray scattering (SAXS), and the length scale of magnetic order is determined from small angle neutron scattering (SANS). These results are correlated with the macroscopic magnetic properties of the assemblies. We find that spin glass-like or mictomagnet behavior dominates when the length scale for structural ordering is less than 300 nm, or about 30 particle diameters.

In the second example we describe FePt nanoparticles that have been suggested for magnetic data storage media. A key advantage of using self-assembled nanoparticle arrays in data storage media would be the high degree of uniformity in the magnetic response. This depends on uniformity in the grain size and interparticle separation and the degree of crystallographic orientation. To be useful for storage media, the arrays must also have long-range structural order. It remains a challenge to prepare nanoparticles with all of these features simultaneously, but significant progress has been made in addressing these problems individually. We report our findings regarding the size-dependence of the fcc to $L1_0$ phase transformation in FePt nanoparticles, and show preliminary results demonstrating the ability to crystallographically align nanoparticles during self-assembly. Finally, we discuss evidence for exchange coupling between nanoparticles through a molecular bridge.

Polymer/Carbon Nanotube Composites: Challenges and Opportunities

Satish Kumar, Georgia Institute of Technology

In the early nineteen twenties, Herman Staudinger began to publish articles asserting that “Polymeric molecules are practically endless chains held together by ordinary chemical bonds”. Even though this idea of practically endless chains appeared foreign to most chemists of that time, these concepts ultimately led to the development of nylon, polyester, isotactic polypropylene, lyotropic polymers such as aramids and benzobisoxazoles, thermotropic polyesters, and gel spun extended chain polyethylene. As a result, polymer and fiber industry went through revolutionary developments, particularly during 1930 – 1980, period. In 1990s, revolutionary developments occurred in other fields such as communication, particularly with the development of internet and wireless communication. The natural question, particularly for someone working in polymers and fibers, is, if we are working in a relatively mature field, as most, recent developments in polymeric fibers may be considered incremental rather than revolutionary. Developments in nanoscale science and technology and its applications to polymers and fibers would suggest that we may be at the initial stages of another revolutionary period which will bring about polymeric and fibrous materials with properties not yet seen. Potential polymeric material developments will be discussed in the light of recent polymer/carbon nanotube composite results.

Time Resolved Spectroscopy of Nitrenes and Nitrenoids in Solution

Matthew S. Platz & Sarah Mandel, Ohio State University

Laser flash photolysis of benzoyl azide and 2,6-difluorophenyl azide in acetonitrile solution produces benzoylnitrene and 2,6-difluorophenylnitrene in their singlet states. The singlet is the ground state of benzoylnitrene but 2,6-difluorophenylnitrene has a triplet ground state. Each of these singlet nitrenes can be detected by electronic absorption spectroscopy and their lifetimes and absolute bimolecular rate constants with organic substrates determined. We have measured the absolute rate constants of reaction of these nitrenes with inorganic salts such as LiCl, LiBr and NaCl to produce nitrenoid species. We will report the first detection of these species using time-resolved using nanosecond time-resolved electronic and vibrational spectroscopy. The lifetimes and reactivity of these species will be reported as well. The spectra will be interpreted with the aid of Density Functional Theory and Time Dependent Density Functional Theory.

Universal Features of Quasi-One-Dimensional Excitons in Pi-conjugated Polymers and Semiconducting Single-Walled Carbon Nanotubes

Sumit Mazumdar, University of Arizona

Following a decade of theoretical and experimental research by many investigators, the exciton model of the electronic structure of pi-conjugated polymers is now firmly established. In particular, exciton theories have been enormously successful in explaining nonlinear optical spectroscopic measurements. In this talk, I will discuss the many-body theory of the electronic structure and photophysics of pi-conjugated polymers. A physical pictorial description of the one-dimensional excitons in these systems will be developed. Following this I will point out that the semiconducting single-walled carbon nanotubes (SWCNTs) can be understood within the same theory. I will show that the low quantum efficiency of the photoluminescence from SWCNTs as well as the discrete structured photoinduced absorptions observed experimentally are both consequences of electron-electron interactions. Taken together, the photophysics of pi-conjugated polymers and SWCNTs provide a deep understanding of excitons in quasi-one-dimensional correlated electron systems.

Patterning a Layer by Tickling the Surface

Rigberto Hernandez & Jeremey Moix, Georgia Institute of Technology

The surfaces of real materials may undergo correlated fluctuations which affect the dynamics of a diffusing adsorbate. The complicated dynamics of this surface is modeled herein through a stochastic potential energy surface which is nonlocal in time and space. Rates and transport across these surfaces have been obtained for one- and two- dimensional coupled to environments ranging from the typical high friction regime down to low friction. In the intermediate to low friction regime relevant to the surface-adsorbate system, the energy from the stochastic surface leads to deviations in thermal equilibrium. Through a naive renormalization of the friction, these deviations have been tamed in previous work. An alternative and more detailed approach requires the use of a space-dependent friction correction. The formalism and comparison between the models will be presented. Enhancements in the rates have been found in one-dimensional aperiodic stochastic potentials. This leads to the possibility of asymmetric transport on two-dimensional stochastic potentials, and it may have implications on the transport of absorbed molecules on two-dimensional surfaces.

Nanoscale Photosynthesis, Molecular Interactions, and the Photocatalytic Evolution of Hydrogen

Elias Greenbaum, B. R. Evans, I. Lee, H. M. O'Neill
Oak Ridge National Laboratory

The photosynthetic reaction centers of photosynthesis are molecular scale photovoltaic structures. They convert light energy into chemical energy by photon absorption followed by voltage generation across the photosynthetic membrane. It is this voltage that is the source of Gibbs energy that drives the thermodynamically uphill reactions of photosynthesis. This talk will focus on recent progress in "wiring" molecular components of the photosynthetic electron transport chain. We have shown that peptide cross-linking of plastocyanin with the oxidizing side of Photosystem I results in increased rates of electron transfer as measured by the rate of photocatalytic hydrogen evolution. The catalyst for hydrogen evolution is photochemically precipitated nanoscale platinum catalyst particles that make electrical contact with the emergent electrons from the Photosystem I reaction center.

Single-Molecule Detection and Imaging

David Ball, The University of Tennessee Space Institute

The detection of individual molecules in solution by laser-induced fluorescence has become an important tool for biophysics research and biotechnology applications. Here, some of our work on detection and imaging of single molecules in solution is reviewed, including experimental configurations for research toward high-speed DNA sequencing and pharmaceutical drug discovery applications. For the latter, to more quickly process slowly diffusing molecules, the sample is caused to flow through a confocal volume into a micron-sized capillary. Evaluation of a prototype 4-channel single-photon detector for multi-channel spectroscopic measurements at the single-molecule level will also be discussed.

Chemical Physics on the Nanoscience Frontier: Update on the CNMS and Research Highlights in Functional Carbon-Based Nanomaterials

Doug Lowndes, Oak Ridge National Laboratory

The construction of ORNL's Center for Nanophase Materials Sciences (CNMS) will be completed in April 2005 and in October 2005 it will be the first of five new DOE Nanoscale Science Research Centers (NSRCs) to begin operation. Research at the CNMS is organized under seven Scientific Themes selected to address challenges to understanding and to exploit ORNL strengths, with the goal of creating a highly collaborative research environment to accelerate discovery and drive technological advances (see <http://cnms.ornl.gov>). This talk will describe the recent and ongoing development of selected CNMS capabilities for nanomaterials synthesis; for imaging, manipulation, and properties measurements in controlled environments; and for theory, modeling, simulation and ultimately design. The latter half of the talk will describe results of recent ORNL research focused on understanding and controlling the synthesis of carbon nanofibers and nanotubes, resulting in varying degrees of control of their position, orientation, and length. Examples will be given of how these nanomaterials can be used to create macroscopic functionality for applications such as field emission of electrons, probing inside of living cells, tips for scanning probe microscopy, and electrically conducting nanotube-polymer composites.

Organic Radical Reactions in Mesoporous Silica: Impact of Pore Surface Confinement

A. C. Buchanan, III, Oak Ridge National Laboratory

Our research is focused on developing a molecular level understanding of the key features that govern the structure, dynamics, and chemical transformations of organic molecules on the surfaces of ordered mesoporous metal oxides over a range of interaction scales from weak hydrogen bonds to strong covalent bonds. Key questions regarding the role of pore confinement, hydrogen bonding, molecular orientation, etc. on thermochemical, photochemical, and catalytic transformations of organic molecules are being addressed. Mesoporous metal oxides with high surface area and controllable morphology, pore size, and pore topology (e.g. MCM-41, MCM-48, and MCM-50 silicas) are being widely investigated because of their many applications in catalysis, separations, and the synthesis of novel nanostructured materials. In this presentation, we describe a method for covalent immobilization of organic molecules in hexagonal mesoporous silicas (MCM-41 and SBA-15) via condensation of aromatic phenols with the surface silanols groups. These hybrid materials have been characterized by a variety of techniques including nitrogen physisorption, diffuse reflectance FTIR, TG-MS, and C-13 NMR. The Si-O-C_{aryl} surface linkage is thermally robust permitting the examination of thermally-induced, free-radical reactions on the surface at temperatures of up to ca. 450°C. However, the linkage can be hydrolytically cleaved for subsequent product analysis. Recent studies of the thermolysis of 1,3-diphenylpropane immobilized in mesoporous silicas with pore sizes varying from 1.7 – 5.6 nm demonstrate that pore confinement can lead to accelerated reaction rates for this radical chain decay mechanism compared with nonporous silicas, and also result in altered product selectivities. The origin of these effects, which are augmented at the smaller pore sizes, will be discussed in the context of the reaction mechanism and the rate-controlling bimolecular hydrogen transfer steps.

Exploring Ultrahigh Magnetic Field Processing of Materials for Developing Customized Microstructures and Enhanced Performance

Gerard M. Ludtka, Oak Ridge National Laboratory

This presentation will cover an innovative and revolutionary research endeavor that is creating the basis for an entirely new research initiative for materials and materials process development. This approach has both scientific and industrial relevance with significant energy savings and environmental benefit ramifications and represents a major step towards achieving materials by design goals. Our experimental and modeling research efforts are clearly demonstrating that phase stability (conventional phase diagrams) can be dramatically altered through the application of an ultrahigh magnetic field. This ability to selectively control microstructural stability and alter transformation kinetics through appropriate selection of the magnetic field strength is being shown to provide a very robust mechanism to develop and tailor enhanced microstructures (even potential bulk nanostructures through accelerated product phase nucleation and transformation kinetics) with superior properties through a more efficient processing technology for a broad spectrum of material applications. The broad goals for this research are to demonstrate and document the influence of ultrahigh magnetic field processing on the phase equilibria and kinetics for ferromagnetic materials and to develop predictive capability based on first principle calculations.

FT-IR of Trace Gases: Atmospheric Analysis and Ionization Products

Jeffrey D. Steill¹, J. Stewart Hager², R. N. Compton^{1,2}, William Blass²

The power of infrared absorption spectroscopy to simultaneously identify, quantify and characterize molecules holds a particular allure for reactive species. Short-lived, reactive gas-phase molecules or ions are amenable to direct spectroscopic study to the degree that we can mitigate the typically low concentrations. Recent attempts at lab-based absorption spectroscopy of reactive molecules and ions from surface ionization will be discussed. Absorption spectroscopy can also be applied outside the laboratory to reactive molecules in the atmosphere, such as O₃. The poor air quality of the local area provides a unique opportunity and incentive. Solar-sourced and open-path absorption spectra provide complementary methods. A spectral line shape analysis is applied to solar-sourced FT-IR spectra to derive the vertical concentration profile of many atmospheric gases, including N₂O, CH₄, CO and O₃. These statistical fitting procedures are improved by the incorporation of the concurrent open-path data into the forward model. Atmospheric open-path (200 m) FT-IR spectra show significant fluxes in trace gases: from 0.36 to 0.28 ppm N₂O, from 1.8 to 1.9 ppm CH₄, and from 1.4 to 0.6 ppm CO. These fluxes are interesting on their own in addition to being important constraints to apply to the solar-spectra analysis.

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Electronic Structure of Dilute Magnetic Semiconductors: A Comparison of the SIC-LSD and the LDA+U Methods

Thomas C. Schulthess (1), L. Petit (1), Walter Temmerman (2), Dridka Szotek (2), G. M. Stocks (1), and W. H. Butler (3)

The Local Density Approximations (LDA) to Density Functional Theory is one of the most successful approaches to compute materials properties from first principles. However, when applied to systems with localized orbitals, such as antiferromagnetic insulators or dilute magnetic semiconductors, the method fails to predict basic ground state properties. Two fairly efficient extensions that are tailored for solids with strongly correlated electrons has been developed over the last two-decade. The first is the LDA+U method, in which an ad hoc on-site Coulomb repulsion for localized orbitals is added to the density functional. This method, which is inspired by the Hubbard model, successfully describes the magnetic and spectroscopic properties of transition metal oxides. The second method is the Self Interaction Corrected (SIC) Local Spin Density (LSD) method, in which the spurious self-interactions of the LDA are subtracted from the density functional. The SIC-LSD is parameter free, successfully describes ground state properties of oxides, but has been criticized for failing to predict the position of localized levels in photoemission spectra. We apply the SIC-LSD method to study the electronic structure and magnetic properties of Mn-doped III-V semiconductors, a new class of materials with intriguing magnetic properties. We compare the results with previous LDA and LDA+U calculations that have so far failed to properly describe the Mn-d orbitals. A proper description of these orbitals is key to understanding of magnetic exchange in these materials. We find, that the SIC-LSD method correctly predicts the p-d exchange strength, and hence Curie temperatures of Mn doped GaAs. We were also able to perform fully self-consistent $B\&B$ -SCF calculation and predict the position of the photoemission peak of the localized levels.

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