

Cluster Science
&
Computational Chemistry
Chemical Physics Workshop 2003

University of Tennessee, Knoxville

ABSTRACTS

Small is Different: Modeling Materials in the Nanoscale Non-Scalable Region

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Investigations of finite aggregates of small sizes and reduced dimensionalities open avenues for systematic explorations of physical factors and unifying principles that underlie the transition from atomic and molecular domain to the condensed phase regime. Such behavior, where the dependence of the behavior of the system on its size is non-scalable with the physical size of the system, but rather where *Small is Different* in an essential way, is emergent in behavior; that is, the exhibited behavior is characteristic of the assembly of particles rather than being a property of the individual constituents, showing interactions between the elementary components of the system. Identification and understanding of the microscopic origins such *emergent phenomena*, are of fundamental importance for the elucidation of the principles of self-assembly and self-selection operative at the nano-scale, as well as of great potential relevance to technological developments at the dawn of the new millennium. These physical and methodological issues will be discussed and illustrated using results obtained through large-scale classical and quantum simulations. Topics will include: (i) formation mechanisms, mechanical, quantized electric conductance, and chemical properties of metal and semiconductor nanowires and their interconnections; (ii) atomic-scale friction, control of friction through modifications of molecular architecture, and nanotribological processes in lubricated junctions; (iii) generation, stability and breakup of nanojets and deposited fractal islands; (iv) nanocatalysis by small gold and palladium clusters, and guidelines for atomic-scale control of catalytic activity; (v) spontaneous symmetry breaking leading to formation of crystallized dots, and quantum-dot-molecules ; (vi) emergence of magnetism on free and surface-supported small palladium clusters; and (vii) charge transport in DNA.

Computer Simulations of Neutral and Charged Water Clusters

K. D. Jordan
University of Pittsburgh

In recent years much progress has been made, with contributions from both theory and experiment, on characterizing the properties of small water clusters. This talk will focus on connections between the topology of the potential energy surfaces and the thermodynamic behavior of the water clusters. It will also address how the properties of the clusters are altered upon addition of a proton or excess electron. In the latter case, a new one? Electron model for including dispersion interactions between the excess electron and the water molecules will be discussed.

Atom Traps Meet Chemical Physics

Linda Young

Argonne National Laboratory

Laser cooling and trapping of atoms are now a mainstay in physics labs worldwide, as atom trapping techniques have become robust and readily accessible. Two Nobel prizes in physics have been awarded in this area in the past 5 years: in 1997 for demonstration of laser cooling and trapping, and, in 2001 for extension of these methods to achieve Bose-Einstein condensation (BEC). In our labs, we have used these techniques to develop atom trap trace analysis (ATTA), a ultrasensitive method capable of single atom detection and part-per-trillion isotopic selectivity. The applications of trace isotope analysis at the ppt level range from dating the polar ice cap to the determination of nuclear charge radii. In this talk, I will briefly review the basics of laser cooling and trapping, discuss alternative techniques for ultrasensitive trace analysis, illustrate the advantages/drawbacks of trace analysis using atom traps with a specific example and have a peek at potential applications.

ESR Matrix Isolation Studies - From Mass Selection to Metal Clusters in Para-Hydrogen

Lon Knight
Furman University

Electron spin resonance (ESR) is a highly sensitive spectroscopic method for gaining direct electronic structure information that can be compared directly with ab- initio theoretical computations. Since most neutral molecules are not radicals, they cannot be detected by ESR, however their corresponding cations contain an unpaired electron making the cation amenable to ESR investigation. The basic physics involved in the trapping of mass-selected cations in solid neon matrices near 4 K has been studied in detail in our laboratory over the past several years. The first successful attempts to couple mass spectrometry, which can produce a wide variety of cation species, with rare gas matrix isolation ESR will be described. Several experimental parameters involved in this trapping process require careful evaluation including the prevention of ion-neutral reactions, the selection of optimum kinetic energy of the cation beam, and the maintenance of macroscopic charge neutrality.

Results for a variety of radical types, including the trapping of neutral metal clusters in para-hydrogen matrix at 2 K, will be summarized.

Design and Synthesis of Molecular-Based Magnetic Lattices

Christopher Landee
Clark University

Increased knowledge of the strategies and techniques of molecular engineering has had a strong impact on the development of novel magnetic materials. Recently developed molecular-based magnets are now being intensively studied for their photo-magnetic properties, spintronics applications, as soluble room-temperature magnets, and as quantum tunneling nanomagnets. This talk will concentrate on new molecular-based quantum antiferromagnets, materials in which quantum fluctuations out of the ground state determine their properties. Examples of one-dimensional, two-dimensional, and spin-ladder lattices will be presented and the correlation between their structure and magnetic properties examined.

Do Baby Crystals Exist?

Puru Jena

Virginia Commonwealth University

Atomic clusters constitute a new phase of matter intermediate between atoms and the bulk. They are the ultimate nano-scale materials where properties can be studied one atom and one electron at a time. The studies of these novel systems have been motivated by two main factors: First, since their properties are size and composition specific, it is expected that a new class of materials with tailored properties can be synthesized by using clusters as building blocks. Secondly, the evolution of their properties as a function of size can illustrate at what point a cluster can be regarded as an embryo of its bulk. This is particularly important since a fundamental understanding of complex processes such as heterogeneous catalysis may be achieved on an atomic scale with these baby crystals as model systems. In addition to providing a general introduction to clusters, this talk will focus on the evolution of the atomic and electronic structure of metal oxide clusters. In particular, I will demonstrate that a tiny cluster consisting of only four tungsten and twelve oxygen atoms bears all the hallmarks of bulk tungsten oxide WO_3 . Similarly, the transition of metallic to semiconducting behavior as a function of oxygen uptake will be shown to occur in clusters at oxygen concentration much below the bulk stoichiometric limit. These results are based on a synergistic approach involving mass distributions under quasi-steady state conditions, photo-electron spectroscopy, and first principles molecular orbital theory and may be applicable in general to a class of systems characterized by strongly covalent or ionic bonding.