ISIS
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Poster Session
Friday, December 7, 2007
University of California, Irvine
1201 Natural Sciences II, 4:00 pm

1. Author(s): Aaron Kushner  
Department of Chemistry, UC Irvine  

**TITLE:** MODULAR DESIGN STRUCTURE: A NEW BIOMIMETIC APPROACH FOR ADVANCED POLYMER AND COMPOSITE MATERIALS  

**Abstract:** The protein titin is a true elastomer that is crucial for the advanced mechanical performance of mammalian muscle. Titin achieves this feat by incorporating sacrificially unfolding domains into the load-bearing fiber. Applying nature’s design of the muscle protein titin to modern synthetic polymers and composites, we can potentially create a new class of advanced materials. We have successfully synthesized a “double-closed loop” (DCL) reversibly unfolding module based on the strong four hydrogen-bond dimerson of the 4-ureido-2-pyrimidone (UPY) motif. Our current project goal is two-fold: 1) incorporate our modular crosslinker in a variety of 3-D network motifs, with both low and high junction densities, and both ordered and disordered architectures, to develop truly strong and tough materials, and 2) further prove our fundamental hypothesis as to the molecular nature of the mechanical enhancement by directly observing the reversible unfolding of our modules via single molecule force-pulling experiments with an AFM. Another project is to develop self-assembly method for linking disulfide nanoparticles that will result in much longer chains of particles by using linking groups that do not terminate chain growth by undergoing undesirable reactions. The plan is to use the four hydrogen bonded 4-ureido-2-pyrimidone (UPY) motif, a group that does not react to form covalent bonds but self-assemble into dimeric form through multiple hydrogen bonds. This will allow the particles to self-assemble into chains with termination reactions that will cut short the growth of the chains.  

2. Author(s): G. Kerenksyaya, I. U. Goldschleger, K. C. Janda, and V. A. Apkarian  
Department of Chemistry, UC Irvine  

**TITLE:** POLYMORPHISM IN Br₂ CLATHRATE HYDRATES  

**Abstract:** Clathrate hydrates are non-stoichiometric compounds, consisting of guest molecules trapped in a lattice of polyhedral water cages. The resurgence of interest in this fascinating class of solids is in part motivated by the recognition of natural deposits of methane hydrates, and their potential global implications with respect to energy and the environment. The structure and composition of bromine clathrate hydrate has been controversial for more than 170 years due to the large variation of its observed stoichiometries. Several different crystal structures were proposed before 1997 when Udachin et al. concluded that Br₂ forms only the tetragonal structure. We show polymorphism in Br₂ clathrate hydrates by identifying two distinct crystal structures through optical microscopy and resonant Raman spectroscopy on single crystals. The two structures are clearly distinguished by the resonant Raman spectra of the clathrated Br₂, which show long overtone progressions and allow the extraction of accurate vibrational parameters.  

3. Author(s): S. Lee, A. Shinde, S. Emori and R. Ragan  
Department of Chemical Engineering & Materials Science, UC Irvine  

**TITLE:** STS AND KPFM STUDIES OF BIMETALLIC CORE SHELL NANOSTRUCTURES  

**Abstract:** Metallic nanoparticles have shown enhanced catalytic activity compared to their bulk counterparts due to changes in electronic properties at the nanoscale. Platinum nanoparticles show no carbon monoxide poisoning for ethylene hydrogenation, while bulk Pt shows an increase in activation energy for the same reaction when exposed to CO. Gold, usually an inert bulk material, shows high catalytic activity at the nanoscale for CO oxidation. Although there are numerous examples of this phenomenon, basic understanding of charge transfer during catalytic reactions is still needed. Challenges in nanoscale catalysis experiments include the fabrication of monodisperse nanostuctures as well as a fundamental knowledge of the electronic properties at this scale. Our group addresses these issues by combining a unique Si-compatible fabrication process for dense ordered arrays of bimetallic core-shell nanostructures with scanning tunneling spectroscopy (STS) and Kelvin probe force microscopy (KPFM). Self-assembled rare earth disilicide nanowires, such as DySi₂ and ErSi₂, are used as templates for Pt and Au nanostructures on vicinal Si(001) and have been characterized previously with scanning probe microscopy. We present an electronic study of the RESi nanowire template as the first phase to completing a comprehensive survey of the entire bimetallic nanomaterial systems.
Abstract:: Mechanical proteins, such as the muscle protein titin, exhibit a remarkable degree of combined toughness, strength, and elasticity, which have yet to be matched by synthetic materials. In an effort to design macromolecular materials having higher-ordered complexity with advanced mechanical properties, we have synthesized a titin-mimicking biopolymer having multiple domain structures. Using protein engineering and chemical conjugation, we designed a polyprotein composed of tandem repeats of a novel enzyme that has no natural load-bearing function. Single-molecule force-extension experiments were carried out which revealed the sequential unfolding of these modules as the polymer is stretched, resulting in sawtooth-patterned curves analogous to those seen in titin. The single-molecule data supports evidence from our steered molecular dynamics simulations showing high resistance to unfolding based on the domain's topology.

50. Author(s):: V. A. Apkarian1, Wilson Ho1, Eric Potma1, Phil Collins1, Nien-Hui Ge1, Doug Mills2, Kieron Burke1, Filipp Furche1, Gui Bazan1, Richard VanDuyne1, Norbert Scherer1
1UC Irvine
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TITLE:: NSF CHEMICAL BONDING CENTER – CASTL
Author(s):: Ping Chu and D. L. Mills
Department of Physics and Astronomy and CaSTL, UC Irvine

TITLE:: COLLECTIVE PLASMON RESONANCES AND THEIR INFLUENCE ON METALLIC NANOSTRUCTURES
Abstract:: We present theoretical studies of the influence of collective plasmon resonances and their influence on enhanced fields, laser induced forces and related issues in selected examples of metallic nanostructures. Our new calculations focus on two nearby dissimilar nanoparticles, and on nanospheres near a planar substrate. We show that when the response of two dissimilar spheres is compared to that of two isolated spheres, breakdown of a selection rule greatly increases the spectral range over which laser fields may couple to collective plasmons. We shall illustrate this with several selected examples. Collective plasmons also influence zero point fluctuations in the electric field near nanostructures; these produce non radioactive transitions and energy level shifts within nearby molecules. We shall present studies of the spatial distribution and frequency spectra of enhanced zero point fluctuations, with the near vicinity of STM tips in mind.

51. Author(s):: Joonhee Lee1, George Nazin2, Qing Huan1, Wendong Xing1 and Wilson Ho2
1Department of Chemistry and CaSTL, UC Irvine
2Department of Physics and Astronomy and CaSTL, UC Irvine

TITLE:: CONSTRUCTION OF A SCANNING TUNNELING MICROSCOPE FOR ENHANCED PHOTON COLLECTION EFFICIENCY
Abstract:: A scanning tunneling microscope (STM) was constructed for optical spectroscopy of single molecules. A parabolic mirror is incorporated into the STM such that the tip apex is positioned on the focal point of the parabolic mirror. Tunneling induced luminescence from Ag-Ag junction shows that photon collection efficiency is significantly enhanced.

52. Author(s):: Ivan Viassous1, Sergei Smirnov1, Zuzanna Siwy1
1University of California, Irvine, New Mexico State University

TITLE:: IONIC FILTER AND NANOFIUIDIC DIODES PERFORMANCE AS A FUNCTION OF THEIR DIMENSIONS
Abstract:: There has been a big interest in preparation of ionic devices such as ionic filters that control transport of ions and charged molecules in aqueous solutions. A bipolar diode example has been constructed by creating a junction between two parts of a nanopore with nega and positive surface charges. A unipolar diode contains a junction between a segment with surf charges and a neutral segment. We investigate the importance of the nanopore length and radius on the performance of different nanofluidic elements. We find that the selectivity of long nanochannel diminishes upon their shortening. Ionic diodes with high rectification ratios can be built only if segments of the pore with positive and negative surface charges are sufficiently long.

53. Author(s):: Dragos E. Constantin and Zuzanna Siwy
Department of Physics and Astronomy, UC Irvine

TITLE:: POISSON-NERNST-PLANCK MODEL OF ION CURRENT RECTIFICATION THROUGH A NANOFIUIDI DIODE
Abstract:: We have investigated ion current rectification properties of a recently prepared bipolar nanofluidic diode. This device is based on a single conically shaped nanopore in a polymer film whose pore walls contain a sharp boundary between positively and negatively charged regions. A semiquantitative model that employs Poisson and Nernst-Planck equations predicts current-voltage curves as well as ionic concentrations and electric potential distributions in this system. We show that under certain conditions the rectification degree, defined as a ratio of currents recorded at the same voltage but opposite polarities, can reach values of over 1000 at a voltage range (~2V, ~2V). The role of thickness and position of the transition zone on the ion current rectification is discussed as well. We also show that the rectification degree scales with the applied voltage.

54. Author(s):: Eric V. Schow1, J. Alfredo Freites2, Douglas J. Tobias1 and Stephen H. White1
1Department of Physics, 2Department of Physiology and Biophysics, 3Department of Chemistry, UC Irvine

TITLE:: THE KVAP CHANNEL IN A LIPID BILAYER: STRUCTURE AND DYNAMICS
Abstract:: Voltage-dependent potassium (Kv) channels open and close in response to change the transmembrane potential. They are composed of a central ion-selective pore domain surrouned by four voltage-sensing (VS) domains. The VSDomains undergo conformational changes associated with the movement of charged amino acid residues (mostly arginines) located in the so-called transmembrane segment. We present results of an atomistic simulation of the archaeabacterial Kv channel in alipid bilayer in excess water. We find that the Arg residues in the S4 transmemembr segment are in a variety of polar solvation environments composed of water molecules, I phosphatse groups, and acidic amino acid side chains. Differences in conformational dynamics suggest that each VS behaves as an independent structural unit. We compare our simulation results to biotin accessibility experiments and LRET measurements in order to validate our model. We assess how different experimental techniques sample the dynamics of the KvAP channel.

55. Author(s):: J.C. Burton, E. Van Cleve, P. Taborek, and J.E. Rutledge
Department of Physics, UC Irvine

TITLE:: A CONTINUOUSLY OPERATING PULSE-TUBE BASED OPTICAL CRYOSTAT FOR TEMPERATURE 0.4 TO 300 KELVIN
Abstract:: We have designed and constructed an evaporative helium-3/helium-4 cryostat capable of continuous operation from 0.4 kelvin. The main temperatures of 0.4 kelvin is achieved using a pulse-tube cooler with 1 watt of cooling power at 4.2 kelvin. Temperatures below 4K are achieved using continuous evaporation of helium-3 or helium-4, and the working fluid car changed during operation. The experimental cell is large enough to accommodate a number of experiments (volume = 3.1 liters), and has five large windows (diameter = 6 cm) for optical access. Current experiments planned for the cryostat include behavior of 2D liquid helium-4 films on al metal and oxidized alkali metal surfaces. The metal films are produced using pulsed-laser deposi from a bulk target in situ. In addition, the hydrodynamic behavior of superfluid helium-4 droplets cesium surfaces will be investigated using high-speed video.
TITLE: NANOTHERMOCOUPLES SYNTHESIZED BY LITHOGRAPHICALLY PATTERNED NANOWIRE ELECTRODEPOSITION

Abstract:: The thermocouple is one of the most commonly used devices for temperature sensing, due to its simplicity and easy integration to electronics. In this work, the dimensions of the thermocouple has been further reduced respect our previous work [1] to lithography from 50 nm to 300 nm by Lithographically Patterned Nanowire Electrodeposition (LPNE) [2]. This new method, based on photolithographic techniques, allows the synthesis of nanowires with a high control of the nanometric dimensions of their cross section, their position and macroscopic shape, and with an electrically continuous layer that can exceed millimeters. The devices present extremely fast response times (<100 ns), high stability over long cycles of heating-cooling (temperature range from 20°C to 120°C), and a stable linearity dependence with time and use.


2. Author(s): Yan He, Zuzanna S. Siwy, Dirk Gillespie, Dezso Boda, Pavel Apel
3. University of California, Irvine
4. JINR, Dubna, Russia

TITLE: ION SELECTIVITY OF POLYMER NANOPORES

Abstract:: Ion selectivity i.e. the ability to transport only one ion and to reject all other ions, is one of the key properties of ion channels. Calcium channels, for example, important in regulation of heart muscle function, can preferably transport calcium ions although monovalent cations, e.g. sodium, are present in extra- and intracellular medium in thousand fold excess to calcium. Selectivity filter of these channels consists of four glutamates, which provide a very high local charge density. The goal of our research is to prepare synthetic nanopores with high density of negative surface charges, and check them for their calcium selectivity. We will show that our nanopores exhibit similar transport properties to calcium biological channels, for example the anomalous mole fraction effect.

10. Author(s): Iuliana E. Sendroui, Ying Han, Robert Corn
Department of Chemistry, UC Irvine

TITLE: FLUORESCENCE AND NANOPARTICLE DIFFRACTION METHODS FOR DNA DETECTION ON PHOTOPATTERNED AMINE-REACTIVE GLASS SUBSTRATES

Abstract:: Oligonucleotides sandwich assays for DNA microarray detection were produced onto photopatterned glass and gold substrates and characterized by means of surface plasmon resonance imaging (SPRI), fluorescence imaging and gold nanoparticle diffraction gratings. Commercial microarray slides based on N-Hydroxysuccinimide (NHS) active ester terminated silane have been successfully photopatterned using UV radiation at 260 nm and a Cr grating mask. Amine-terminated single-stranded DNA (D1) probes were selectively attached onto the glass slides and hybridized with a target ssDNA sequence (DM), half complementary to D1. SPR imaging was used to monitor in real time each hybridization step. To create a fluorescence-based microarray, a second hybridization was performed using a fluorescently labeled ssDNA (D2) complementary to the second half of the target ssDNA. Fluorescence imaging experiments showed bright emission down to a concentration of 10 nM of the target DNA. Similarly, DNA sandwich assays for diffraction gratings detection method used DNA modified gold nanoparticles as the D2 complement. Diffraction gratings spots were observed for target DNA concentrations as low as 10 pM.

18. Author(s): Kartarien U. Arvia, Maria J. Kriscn, Matthew A. Brown, Douglas J. Iodias, John C. Hemminger, Markus Ammann, Hendrik Bluhm, David E. Starr
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2Paul Scherrer Institute
3Lawrence Berkeley National Laboratory

TITLE: THE EFFECT OF AN ORGANIC SURFACANT ON THE LIQUID-VAPOR INTERFACE OF AN ELECTROLYTE SOLUTION

Abstract:: The addition of 1-butanol to an aqueous potassium iodide solution modifies the interfae profile of ions at the liquid - vapor interface. Our experiments probe atomic composition at the interface using ambient pressure x-ray photoelectron spectroscopy. Photoelectron kinetic energies varied to produce a depth profile of the liquid - vapor interface. Surface enhancement of ion anions, an effect observed in aqueous potassium iodide solution, disappears in the presence of butanol, a surface active alcohol. Molecular dynamics simulations of butanol in an aque electrolyte solution exhibit the same effect. Radial distribution functions calculated from simulations show that butanol appears to interact with both the anion and the cation; this is likely to the basis for the observed changes in the ion distribution in the presence of the organic. Insight ion behavior at mixed organic/aqueous liquid surfaces is crucial for understanding the chemist atmospheric aerosols, which frequently contain mixtures of water, electrolytes, and organics.

21. Author(s): Matthew R. Powell, Michael Sullivan, Ivan Vlassiouk, Dragos Constantin, Olivier Sudre, Craig C. Martens, Robert S. Eisenberg, Zuzanna S. Siwy
1Department of Physics and Astronomy, UC Irvine
2Teledyne Scientific Co.
3Department Chemistry, UC Irvine
4Rush Medical College, Chicago

TITLE: ION CURRENT OSCILLATIONS CAUSED BY FEMTOFLITER VOLUME PRECIPITATION IN A NANOPORE

Abstract:: The fixed negative surface charges inside single conical polymer nanopores result in transport properties not encountered in micrometer-scale counterparts. The nanopores described here are created with the track etching technique resulting in a conical geometry having a 1 mm opening of hundreds of nanometers and a small opening of several nanometers. A new phenomenon is presented detailing an oscillating ionic current through our conical nanopore when a small amount of a divalent cation is added to a buffered monovalent ionic solution. An ionic current enhancer brought on by the superposition of the electric field from the fixed negative surface charges and externally applied electric field causes a formation and redisolution of nanoprecipitates temporarily block the ionic current through the pore. This oscillating system could be used as a model for studying nonlinear electrochemical processes and early stages of crystallization.

23. Author(s): A. A. Maradudin, T. A. Leskova, I. Simonsen
1Department of Physics and Astronomy and Institute for Surface and Interface Science
2Laboratoire Mixte CNRS/Saint-Gobain and Department of Physics, Norwegian University Science and Technology

TITLE: SURFACE ELECTROMAGNETIC WAVES ON TWO-DIMENSIONAL DOUBLY PERIODIC PERFECTLY CONDUCTING SURFACES

Abstract:: It is well known that the planar surface of a semi-infinite perfect conductor does not support a surface electromagnetic wave. It supports a surface skimming bulk electromagnetic wave that is not bound to the surface. This wave is "unstable" in the sense that even a slight change of boundary condition on the perfectly conducting surface converts it into a surface wave or into a surface wave and a surface shape resonance, both of which are bound to the surface. In this paper we study the propagation of surface electromagnetic waves on a two-dimensional perfectly conducting surface that is doubly periodically rough. We derive the Rayleigh equation for the electric field in the vacuum region above a two-dimensional rough perfectly conducting surface. We then calculate the dispersion relation of the surface electromagnetic waves in the case where the surface is represented as a square array of hemispheres. We show that it is possible to modify the dispersion curves of surface waves by varying the lattice parameter of the surface structure and the size and shape of the units forming that structure. In particular we show that for a sufficiently strong modulation of surface a second, higher frequency, branch of the dispersion curve enters the non-radiative region and can give rise to an absolute band gap between the two branches.
TITLE:: OZONE OXIDATION OF SELF-ASSEMBLED MONOLAYERS ON SILICON SURFACES

Abstract:: Airborne particles have effects on human health, visibility and the chemistry of the atmosphere. A major concern, but also largely uncertain, is the impact of particles on global climate. Part of this uncertainty is the lack of understanding of the nature of the organic component. This deficiency includes the chemical speciation and the distribution of the organics between the surface and the bulk of liquid particles, as well as changes due to oxidation during transport in the atmosphere. Vinyl-terminated self-assembled monolayers (SAMs) on silicon substrates were used as proxies for the organics adsorbed on airborne dust. Ozonolysis of alkene SAMs leads to the formation of large aggregative compounds which do not increase the uptake of water as previously assumed. FTIR, AFM, SEM, Auger microprobe, and TOF-SIMS were used to study the surface composition and morphology after oxidation. Atmospheric implications for the oxidation of alkenes on airborne dust particles are discussed.

23. Author(s): Matthew Shindel, Prof. Szu-Wen Wang, Prof. Daniel Mumm
   Dept. of Chemical Engineering and Material Science, UC Irvine

TITLE:: FABRICATION OF NANOPARTICLE ARRAYS ON PROTEIN CRYSTAL TEMPLATE

Abstract:: The protein streptavidin has the ability to crystallize on solid supported lipid layers. Prior work has demonstrated that such crystals have tunable macroscopic and molecular (i.e. lattice) morphologies. These morphologies are suggested to have the effect of stratifying the surface of the two-protein molecule on its free surface allows this system to act as a template for arrays of inorganic nanoparticles. This work investigates the ability of streptavidin crystals to generate ordered arrays of gold colloids through specific streptavidin-biotin linkage (KA ~ 1015 M-1). Streptavidin crystals were formed on mica supported phospholipid bilayers. Biotin moieties were conjugated to the surface of 20nm gold nanoparticles allowing for specific attachment of particles to the crystal template. The particle functionalization process was analyzed with FTIR and UV-Vis spectroscopy and array samples were imaged with SEM and AFM.

24. Author(s): Danny Wan, Brett R. Goldsmith, Philip G. Collins
   Department of Physics and Astronomy, UC Irvine

TITLE:: CNT GROWTH THROUGH COMPUTER CONTROLLED CVD

Abstract:: Integration of carbon nanotubes (CNTs) into feasible devices for nanoelectronic circuits, chemical and biological sensing, and individual defect site characterization first requires a scalable method of CNT production. Chemical vapor deposition (CVD) nanotube growth has been shown to be a high yield and reproducible method for growth. Diameter specific nanotubes can be grown using catalysts. We also demonstrate computer controlled CVD growth of CNTs by way of communication through data acquisition card and show images of our recent efforts in using this method.

25. Author(s): Kapil Krishnan, Michael Dennin
   Department of Physics and Astronomy, UC Irvine

TITLE:: REVERSIBLE PLASTICITY

Abstract:: A fundamental assumption in our understanding of material rheology is that when microscopic deformations are reversible, the material responds elastically to external loads. Plasticity, i.e. dissipative and irreversible macroscopic changes in a material, is assumed to be the consequence of irreversible microscopic events. In this poster, we show direct evidence for the coexistence of reversible and irreversible plastic events at the microscopic scale in both experiments and simulations of two-dimensional foam. The simulations demonstrate a link between reversible plastic rearrangement events and pathways in the potential energy landscape of the system.

26. Author(s): I. U. Goldschlegler, V. Senekerimyan, and V. A. Aplakian
   Department of Chemistry, UC Irvine

TITLE:: PORTRAIT OF QUANTUM DISSIPATIVE OSCILLATOR: BR2 DOPED ICE

Abstract:: Spectrally-resolved transient grating measurements of Br2 enclathrated in ice allow direct imaging of vibrational densities. *Error! Objects cannot be created from editing field codes.* A single image of a quantum coherent oscillator emerges after a period of strongly coupled system-bath dynamics, during which the system evolves in a continuum of states and undergoes extensive dissipation. The images can be manipulated to extract temporal and spatial vibrational coherence that clearly show eigenstates deeply buried in the continuum of states, which cannot be directly observed due to electronic dephasing (decoherence). The quantum nature of the oscillator is, for the first time, established by resolving wavefunctions imprinted in the spatial coherence. The observables characterize a molecule enclathrated in a cage that mechanically and electrically insulates it from rest of the solid (amorphous ice).
TITLE:: SELF ASSEMBLY OF GOLD NANOPARTICLES ON DIBLOCK COPOLYMER TEMPLATES FOR USE AS BIOMOLECULAR SENSORS

Abstract:: Nanoscale metallic structures have been utilized in field-enhanced chemical and biological detection devices since closely spaced noble metal nanostructures have the capacity to achieve single-molecule level detection limits resulting from Surface Enhanced Raman Scattering (SERS). By fabricating arrays of noble metal nanoparticles having controlled size and shape on a self-organized polymer template, we have developed a surface with a measured preliminary SERS enhancement factor of the order of 10^7. These surfaces are fabricated by forming a polymer template of polystyrene-b-poly(methyl methacrylate) (PS-b-PMMA) with a fractional domain of 26.24% PMMA organized in 20 nm diameter hexagonally packed PMMA cylindrical regions and functionalized with terminating primary amine groups. Chemically synthesized gold nanoparticles, measured at 20 nm diameter using dynamic light scattering (DLS) techniques and scanning electron microscopy (SEM), were attached to these surface amine regions via an organic ligand on the nanoparticle surface.

16. Author(s):: K. Unal, S. Balci and H. K. Wickramasinghe
Department of Electrical Engineering & Computer Science, UC Irvine

TITLE:: SURFACE ELECTROPHORESIS ON ATOMIC FORCE MICROSCOPE PROBE TIPS

Abstract:: An AFM is tailored to perform ultra-fast electrophoretic mobility measurements on populations of 0.1 zeptomoles (10-22 moles) on the surface of a probe tip. The driving force is a large electric field applied over the length of an AFM tip that results in enhanced differential mobilities stemming from the confinement of the water layer on the tip surface. DNA oligonucleotides exhibit migration times in the order of ms, ~5 orders of magnitude faster than in conventional capillary electrophoresis.

17. Author(s):: F. Yang, 1 C. Xiang, 1 S. C. Kung, 1 A.G. Güell, 2 J. Kagan, 2 R. M. Penner 1,2
1 Department of Chemistry and Institute for Surface and Interface Science, UC Irvine
2 Department of Physical Chemistry, University of Barcelona

TITLE:: HYDROGEN SENSING WITH A SINGLE PALLADIUM NANOWIRE

Abstract:: Hydrogen sensors were fabricated from single palladium nanowires. These nanowires, prepared by Lithographically Patterned Nanowire Electrodeposition (LPNE) were rectangular in cross-section with widths and thicknesses of 30 to 500nm (width) and 10 to 40nm (thickness). The wire length could exceed 1mm. Using a four-point evaporated gold contact, hydrogen sensors were fabricated from a 100 m section of these nanowires. These palladium nanowires were characterized by AFM, SEM, TEM and XRD. Hydrogen sensors of same width (~50nm) and different thickness (10 to 40nm) were exposed to hydrogen gas with a concentration range of 0.02 to 10%. We compare the properties of these nanowires for detecting hydrogen with that of sensors based upon pure palladium films of the same thickness. Both response-time and relative resistance change were investigated at room temperature.

18. Author(s):: Attila Cangi, Peter Elliott, Donghyung Lee, and Kieron Burke
Departments of Chemistry and of Physics, UC Irvine

TITLE:: SEMICLASSICAL ORIGINS OF DENSITY FUNCTIONALS

Abstract:: Since its foundation almost 80 years ago, Density Functional Theory (DFT) has gained the status of a successful, widely-used theory in different areas of chemistry and physics. To improve the predictions of DFT and apply it to ever larger systems we have to approximate the components of the energy of a given system accurately and computationally inexpensively. We show how functionals can be improved by analyzing the semiclassical limit of large particle number [1, 2].


19. Author(s):: D. A. Taggart, T. Tang, S. C. Kung, U. Xiang, F. Tang, A.G. Güell, M. A. Brown,1 J. C. Hemminger, 1 R. M. Penner 1,2
1 Department of Chemistry and Institute for Surface and Interface Science, UC Irvine
2 Department of Physical Chemistry, University of Barcelona

TITLE:: THERMOELECTRIC NANOWIRES OF Bi2Te3 AND PbTe

Abstract:: The theoretical understanding of thermoelectric materials has advanced in dramatic fashion over the last eight years. One important prediction of this theory is that one-dimensional nanowires for enhanced electronic conductivities and/or enhanced thermal conductivities relative to bulk materials. Theoretical predictions have been observed in nanostructured materials, but not yet isolated nanowires. One reason for the absence of data here is the difficulty in making high-quality and isolated nanowires that are microns in length. We have sought a new method for prepaing nanowires of thermoelectric materials that circumvents the measurement problem. In presentation, we focus attention on the synthesis of Bi2Te3 and PbTe nanowires. The polycrystalline nanowires were grown via the LPNE (Lithographically patterned nanowire electrodeposition) method which involves the patterning, by photolithography, of a metal nanowire electrode on a glass or oxidized silicon surface, and the subsequent electrodeposition of the nanowire at this electrode. After nanowire growth, the metal electrode and remaining photoreist selectively removed, leaving the nanowire supported on a dielectric. The lateral dimensions of the nanowire can be controlled over the range from 80 to 500 nm, and the electronically continuous layer of the nanowires can exceed millimeters. This means that four-contact conductivity measurements can be carried out using evaporated nickel contacts, and we describe the outcome of the measurements. The structural and chemical characterization of these nanowires are discussed in detail with attention to the tuning the composition via the composition of the plating solution and electrodeposition parameters.

Acknowledgement: This work was supported by the UCI School of Physical Sciences Center for Solar Energy.

20. Author(s):: Matthew Aggleton (Taborek group)
Department of Physics, UC Irvine

TITLE:: ULTRA-HIGH VACUUM CRYOTRIBOLOGY OF SOLID AND LIQUID LUBRICANTS

Abstract:: We have used a sliding block tribometer (described in J.C. Burton, P. Taborek, and Rutledge, TRIBOLOGY LETTERS 23, 131, 2006) to measure the temperature dependence of kinetic friction coefficient of various materials; including single crystal diamond on various types of CVD diamond films, steel on molybdenum disulfide + titanium thin film, and steel on synthetic hydrocarbon oil lubricant. We are primarily interested in the response of the coefficients of friction to pressure and temperature changes. These measurements have been performed across pressures from 2 0000 psi to 6 700 psi, temperature from -200 to 300 Kelvin. Microcrystalline diamond, nanocrystalline, and diamond-like carbon, although compo of the same building blocks, exhibit vastly different coefficients of friction under varying pressure and temperature conditions. We have also studied other films and liquid lubricants under these same pressure and temperature conditions, results of which will be presented.

21. Author(s):: Neelanjana Sen Gupta (Tobias group)
Department of Chemistry, UC Irvine

TITLE:: USING MOLECULAR DYNAMICS SIMULATIONS TO INTERPRET THE SPECTRAL SIGNATURES OBTAINED FROM TWO-DIMENSIONAL INFRARED SPECTROSCOPY OF A HELIC OCTAPEPTIDE

Abstract:: We present structural analysis and 2DIR spectra of the amide-I vibrational mode of alpha Carbon-methylated peptide; -methylated peptide solvated in deuterated chloroform. Spectral calculations from MD simulation trajectories are compared with 2DIR experiments in parallel double-crossed polarization configurations. Structural determination of simulated conformers is done by hydrogen bond analysis and by dihedral angle analysis of each residue. It is seen that molecular dynamics simulations drive the system to unoccupied regions in the Ramachandran space, gh rise to extra features in the spectra. Positional restraints are useful in obtaining trajectories that reproduce the experimental spectra. The spectra calculated under the double-crossed polarization have greater sensitivity to structural changes than those under the parallel polarization. This st correlates the 2DIR spectral features to details of helical secondary structure, compares res obtained from different methods of spectral calculation with experiments, and points out the deficit current force fields.