2008 Joint Meeting of the APS Ohio-Region Section, the AAPT Southern Ohio Section, and the ACS Dayton-Section
Dayton, Ohio
http://meetings.aps.org/Meeting/OSF08/
1:45PM A1.00001 Spectroscopic indicators of life on other planets JAMES F. KASTING, Department of Geosciences, Penn State University — Astronomers have now identified over 300 extrasolar planets orbiting nearby stars. Most of these planets have been found by using ground-based instruments to measure Doppler shifts in the spectrum of the parent star. For stars similar to our Sun, this method is unable to find planets as small as Earth. Within the next two (three?) decades, however, NASA hopes to launch space-based telescopes that will be able to search directly for extrasolar planets. NASA’s planned Terrestrial Planet Finder (TPF) missions, will look for Earth-like planets around nearby stars and, if they exist, provide spectroscopic information on their atmospheres. TPF-C will be a coronagraph that operates in the visible/near-IR. A variant of this idea, called TPF-O, would replace the internal coronagraph with a free-flying occulting disk. TPF-I is envisioned as a free-flying interferometer operating in the thermal-IR. On a planet like modern Earth, TPF-C or TPF-O should be able to see absorption bands of O2, H2O, and possibly O3. TPF-I would be able to see CO2, H2O, and O2. Both O2 and O3 are considered to be good indicators of life for planets orbiting within the liquid water habitable zone of their parent star. Even better evidence for life would be the simultaneous observation of O2 (or O3) and a reduced gas such as CH4 or N2O. That may not be possible with a first-generation TPF instrument but should ultimately be possible in the more distant future.

2:45PM A1.00002 Ultrafast dynamics with laser-produced soft X-rays STEPHEN R. LEONE, University of California and Lawrence Berkeley National Laboratory — Laser-produced high order harmonics are used to probe chemical dynamics of atoms and molecules on femtosecond timescales. Two basic methods are developed, ultrafast transient absorption and photoelectron spectroscopy. The high order harmonics are produced with a 800 nm Ti:Sapphire laser focused into a capillary or rare gas jet. Both inner shell core levels and outer shell valence states are investigated. The transient absorption of xenon ions produced by high field ionization of neutral xenon atoms is probed by core level spectroscopy. The alignment of the vacancy created in forming the ion is measured as a function of pump-probe delay by promotion of an inner d electron to the vacancy in the outer shell. Small molecules are excited to repulsive dissociative states and individual harmonics are used to obtain time-resolved photoelectron spectra. A wave packet on the dissociative state of bromine molecules is detected, as well as the production of atoms at longer time delays. By the use of velocity map imaging, the angular distributions of outgoing photoelectrons are analyzed for selected excited states of He atoms, providing new information about the relative phases and matrix elements for photoionization into the outgoing d and s waves.

4:30PM - 4:30PM — Session P1 Poster Session (16:30-18:00) Student Union E 156

P1.00001 Design optimization of passive micromixers with fractal surface patterning PETRU FODOR, MATTHEW ITOMLENSKIS, MIRON KAUFMAN, Cleveland State University — Relief patterning of the surface of microchannels has been actively pursued as a method of promoting mixing in systems with a low Reynolds number (<100). For example, structures such as the staggered herring bone (SHB), which consists of periodic grooves and ridges distributed along the channel length, improve mixing by inducing counter – rotating helical flows in pressure driven systems. In this work, we explore computationally using the COMSOL Multiphysics Package and its Chemical Engineering Module, the possibility of enhancing the mixing quality of two fluids within a microchannel by employing a Weierstrass fractal function with different fractal dimensions to produce a non-periodic pattern of grooves and ridges on the channel bottom. The designs are optimized with respect to two geometrical parameters: i.e the distances between the ridges and the position range of their tip along the width of the channels. The quality of the mixing between two fluids is analyzed numerically using an entropic measure for the binary fluid system, and is compared with the performance of SHB designs with similar geometrical parameters. The results show that the mixing efficiency associated with Weierstrass function based designs is consistently better than for the SHB counterparts.

P1.00002 Terahertz Radar for Remote Measurement of Vital Signs CARLA BENTON, ERIK BRYAN, DOUGLAS T. PETKIE — A radar system operating at 228 GHz was used for measuring the displacement of a subject’s chest wall due to respiration and heartbeat. Using various signal processing techniques, the signal was cleaned and the respiration rate and heart rate were extracted from the signal. The radar has been able to produce accurate results at a variety of distances and recent improvements to the system and the signal processing have increased its operating range and accuracy.

P1.00003 Stellar Surface Imaging of LO Pegasi RACHEL DECKER, Ohio Wesleyan University, CONRAD MOORE, Bucknell University, ROBERT HARMON, Ohio Wesleyan University — We present images of dark starspots on the surface of the K8 main-sequence star LO Pegasi. CCD camera images of the star and surrounding field were acquired through B, V, R and I filters at Perkins Observatory in Delaware, OH on clear nights in June and July, 2008. The images were dark-subtracted and flat-fielded and then aperture photometry was performed to yield light curves through each of the four filters. These light curves were then simultaneously inverted via an algorithm devised by one of us (Harmon) so as to yield images of the spots based on the rotational modulation they produced in the light curves. The use of multiple filters significantly improves the latitude resolution of the reconstructions. Comparison of our results with results from 2006 and 2007 shows that the spot structure was more complex in 2008 than in the prior years.

1 This research was funded by the OWU Summer Science Research Program and the NSF REU Program.

P1.00004 Conditional Bell-state discrimination by direct photodetection of emission from a pair of atoms RICHARD WAGNER, JAMES CLEMENS, Department of Physics, Miami University — We report on the performance of a protocol for conditional Bell-state discrimination by means of direct photodetection of the spontaneous emission from a pair of atoms. The performance is characterized by the fidelity of the teleportation of an unknown quantum state from one of the atoms onto the photon number states of a cavity field mode. We find a fidelity approaching unity for atomic separation much less than an emission wavelength with a success probability of 25%. The fidelity is reduced from the ideal value when imperfect photodetection efficiency is taken into account but still exceeds the value of 2/3 predicted for a classical teleportation protocol.

P1.00005 Activation energy of water desorption from guanosine. MEGAN SMITH, SCOTT LEE, University of Toledo — The interactions of the nucleic acids with their water of hydration are of fundamental importance and still imperfectly understood. As an initial effort, we have studied a component of RNA: the nucleoside guanosine (rG), composed of the ribose sugar and the guanine base. The interactions of the water of primary hydration with rG have been studied via thermogravimetric measurements and differential thermal analysis. These data yield the activation energy for the desorption of the water of primary hydration from rG.
Investigations into the mechanical properties of fibrinogen using molecular simulations. AMIT DONGOL, RUXANDRA DIMA, University of Cincinnati — Fibrinogen, a hexameric molecule, is the main component of a blood clot [1]. The clots are under the action of large mechanical forces during blood flow or at the site of the wound. Hence it is crucial to study the mechanical properties of fibrinogen, which are likely to be responsible for the force response of the clots [2]. To understand the molecular origins of the mechanical properties of fibrinogen, we performed Langevin simulations of a minimalist polymer model of this molecule. Our model [3] enables us to simulate the force-induced unfolding of fibrinogen at experimental loading rates. Our simulations revealed critical unfolding forces in the range of 100 pN in accord with experimental results. By surveying the structures of the various metastable intermediates, we map features of the complex energy landscape of fibrinogen which are at the origin of clot elasticity.


Substrate protein recognition mechanism of archaean and eukaryotic chaperonins. POOJA SHRESTHA, GEORGE STAN, University of Cincinnati — Chaperonins are double ring-shaped biological nanomachines that assist protein folding under non-permissive conditions. Spectacular conformational changes take place within each chaperonin ring using energy derived from ATP hydrolysis. These changes result in transitions from open to closed chaperonin ring via partially closed state. Substrate proteins bind to the open chaperonin ring and are encapsulated within the closed cavity. We focus on the substrate protein recognition mechanism of group II chaperonins. We predict substrate protein binding sites using structural and bioinformatic analyses of functional states. Based on large changes in solvent accessible surface area and contact maps we glean the functional role of chaperonin amino acids. During the transition between open to closed chaperonin ring, the largest change in accessible surface area is found in two helices located at the cavity opening. Based on these calculations and the bioinformatic prediction of protein interaction regions we suggest that these two helices constitute the substrate protein binding site.

Intermediate interactions of reduced nicotinamide adenine dinucleotide (NADH) in solution. JOSHUA JASENSKY, M. JUNAID FAROOQI, PAUL URAYAMA, Miami University — Nicotinamide adenine dinucleotide (NAD+/NADH) is a coenzyme involved in cellular respiration as an electron transporter. In aqueous solution, the molecule exhibits a folding transition characterized by the stacking of its aromatic moieties. A transition to an unfolded conformation is possible using chemical denaturants like methanol. Because the reduced NADH form is fluorescent, the folding transition can be monitored using fluorescence spectroscopy, e.g., via a blue-shift in the UV-excited emission peak upon methanol unfolding. Here we present evidence of interactions between NADH molecules in solution. We measure the excited-state emission from NADH at various concentrations (1-100 μM) in MOPS buffer, pH 7.5; 337-nm wavelength excitation). Unlike for the folded form, the emission peak wavelength of the unfolded form is concentration dependent, exhibiting a red-shift with higher NADH concentration, suggesting the presence of intermolecular interactions. An understanding of NADH spectra in solution would assist in interpreting intercellular NADH measurements used for the in vivo monitoring cellular energy metabolism.

1. Supported by an award from Research Corporation. JJ was supported by Miami University’s Undergraduate Summer Scholars program.

Long-time Behavior of Surface Electromyography Time Series. BRIAN VYHNALEK, Physics Dept, Cleveland State University, ULRICH ZURCHER1, MIRON KAUFMAN, Physics Dept, Cleveland State University, PAUL SUNG, Health Sciences Dept, Cleveland State University — We have previously reported that the mean-square displacement from the sEMG time series increases as time

Integrating with the number of the group cannot be more than the unit should be carried out. Then the hyperboles have smooth shape without breaks. It confirms that any element of the Periodic Table was considered at the numerator. Now we expand the law: we enter the groups OH, CO3, SO4 and the others into the hyperboles is that the contents of substance of a specific chemical element should take the quantity of one gram-atom. Earlier, there in the equation Y=K/X

Correlation. HPC microgels undergo a similar transition in which, however, microgel clusters stay intact below and above T

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Effect of Polymer Concentration and Cross-linking Density on Microgel Size and Shrinkage Capacity. KIRIL STRELETZKY, IMAAN BENMERZOUGA, JOHN MCKENNA, Cleveland State University — Hydroxypropylcellulose (HPC) is a polycsaccharide with temperature dependent water solubility. HPC chains can be chemically cross-linked into stable nanoparticles called microgels. The structure and dynamics of microgels depend on polymer and salt concentration, crosslinking density, and solution temperature. HPC has easily accessible lower critical solution temperatures. At T,=41°C, HPC in solution undergoes a reversible transition at which chains form metastable clusters that fall apart when temperature is lowered below Tc. HPC microgels undergo a similar transition in which, however, microgel clusters stay intact below and above Tc. In this transition microgels shrink/swell on average by a factor of eight, a property with potential for application in targeted drug delivery. Dynamic Light Scattering was used to study microgels in thermal equilibrium. Due to the complexity of microgel spectra the line shape analysis algorithm was employed. Comparison of differently synthesized HPC microgels revealed that higher polymer concentration results in smaller microgels with lower shrinking capacity. The effective cross-linking density that yields relatively monodisperse microgels was determined. The angular dependence of scattering demonstrated that microgels are largely spherical particles. Finally, studying microgels at different temperatures allowed to monitor the shrinking/swelling behavior.

The Law of Hyperboles for Chemical Compounds. ALBERT KHAZAN — The essence of the law of the hyperboles is that the contents of substance of a specific chemical element should take the quantity of one gram-atom. Earlier, there in the equation Y=K/X

The rotational spectrum of deuterated nitric acid. APRIL HEDDINGS, DOUGLAS T. PETKIE, Wright State University — The terahertz rotational spectrum of many small fundamental gas-phase molecules provides an absolutely specific spectral fingerprint and insight into the intramolecular forces through the fitted rotational and vibrational constants. We are currently assigning and fitting the measured rotational transitions in several of the lowest lying, thermally populated, vibrational states of deuterated nitric acid. We will describe the general characteristics of the spectrum and compare the rotational and centrifugal distortion constants of each state to those of the normal species.
P1.00013 The Fractional-Linear Function in the Hyperbolic Law, ALBERT KHAZAN — The maintenance of any element in a chemical compound decreases with increase of the molecular weight under the equipotential hyperbolic law Y=K/X (1). However the size (1-Y) increases according to the equation 1-Y=K/X or Y = (X-K)/X (2). This function refers to as fractional-linear one, and after transformations turns to the equation of an equipotential hyperbola whose center is displaced from the beginning of the coordinates about (0; 0) in a point with (0; 1). Hence, the valid axis on which there tops of new hyperboles are, pass perpendicularly to the axes of the equation (1). We shall enter names for hyperboles: (1) - "straight one." (2) - "adjacent one." Their directions are mutually opposite in the point Y=0.5 of crossing of each pair; this line is an axis of symmetry for all the hyperboles; the absissa is equal to the double nuclear weight of any element (2K). Coordinates of other crossing points of the hyperboles have following parameters: X = (K1+K2), Y1 = [K1/(K1+K2)], Y2 = [K2/(K1+K2)]. At the last element the curves designate the borders of the existence of possible chemical compounds (Progr. Phys., 2007, 1, 38; 2, 83; 2, 104; 2008, 3, 56).

P1.00014 Field deployable microcantilever based chemical sensing: discrimination between H2O, DMMP and Toluene, E.J. THORESON, ITT AES, NSTA, Dayton, OH 45431, T.H. STIEVATER, W.S. RABINOVICH, M.S. FERRARO, N.A. PAPANICOLAOU, R. BASS, J.B. BOOS, J.L. STEPNOWSKI, R.A. MCGILL, Naval Research Laboratory, Washington, DC 20375 — Low cost passive detection of Chemical Warfare Agents (CWA) and being able to distinguish them from interferents is of great interest in the protection of human capital. If CWA sensors could be made cheaply enough, they could be deployed profusely throughout the environment intended for protection. NRL (Naval Research Labs) has demonstrated a small sensor with potentially very low unit cost and compatible with high volume production which has the ability to distinguish between H2O, DMMP, and Toluene. Additionally, they have measured concentrations as low as 17 ppb passively in a package the size of a quarter. Using the latest MEMS technology coupled with advanced chemical identification algorithms we propose a development path for a low cost, highly integrated chemical sensor capable of detecting CWA's, Explosives, VOC's (Volatile Organic Chemicals), and TIC’s (Toxic Industrial Chemicals). ITT AES (Advanced Engineering & Sciences) has partnered with NRL (Naval Research Labs) to develop this “microharp” technology into a field deployable sensor that will be capable of remote communication with a central server.

P1.00015 Introducing Quantum Mechanics into General Chemistry, IWONA POPKOWSKI, HAFED BASCAL, University of Findlay — Periodicity has long been recognized as the tool that chemists can use to bring some order to investigating the chemistry of more than one hundred elements. Such studies provide useful tools for understanding a wide array of chemical principles. The advances in computational chemistry make it possible to study and teach such trends with hands on approach. In this study we utilize recently acquired software Spartan Pro to illustrate theoretical measurements of bond length, bond angle and dipole as compared to experimental data. We constructed a matrix of values obtained from the theoretical calculations and obtained trends in bond length, bond angle and dipoles for the several periodic groups.

P1.00016 Measuring dn/dc of HPC polymer and microgel solutions, KRISTA FREEMAN, KIRIL STRELETZKY, Cleveland State University — The refraction process is the basis of light scattering experiments on transparent solutions where light refraction depends on spontaneous concentration fluctuations in solution caused by molecular Brownian motion. The specific refractive index increment (dn/dc), the change in index of refraction with concentration, is essential for static light scattering (SLS) experiments on polymer solutions. With a reliable value for dn/dc, SLS yields radius of gyration and molecular weight of the polymer, and second virial coefficient. This study focuses on determining dn/dc values of hydroxypropylcellulose (HPC) polymer and microgel solutions. Precise calibration of the Brice-Phoenix differential refractometer (BP) was necessary to attain accurate values for dn/dc. Using the BP, HPC solutions were studied at a range of concentrations, molecular weights, wavelengths, temperatures, and filtration protocols. Through the course of the study it was determined that dn/dc of HPC polymer is independent of temperature in good solvents, slightly dependent on molecular weight, inversely proportional to wavelength squared, and sensitive to polymer solution’s filtration protocol. HPC microgel testing produced dn/dc values one order of magnitude larger than the dn/dc of HPC polymer solutions and did not support the expected wavelength dependence.

P1.00017 Monte Carlo Simulation Study of Lattice Gas Diffusion in a Box Fractal1, DANIEL P. KNOWLTON, Dept. of Physics, Doane College, Crete, NE, JAMES L. JOHNSON, Dept. of Mathematics, Doane College, Crete, NE, CHRISTOPHER D. WENTWORTH, Dept. of Physics, Doane College, Crete, NE — In this investigation we study a simple model of diffusion of a concentrated lattice gas in a box fractal structure. The model involves a fixed concentration of particles that undergo random hopping to nearest-neighbor sites with equal probability. The particles do not interact except that double-occupancy of a lattice site is not allowed. The particles move in a lattice of box fractal structure, which has a fractal dimension of 1.465. The mean-square displacement of a tracer particle as a function of time is calculated from the simulation. The simulation suggests anomalous diffusion occurs in this lattice structure.

1Support provided by the Doane College Undergraduate Research Program

P1.00018 Diffusion of a Concentrated Lattice Gas in a Regular Comb Structure1, PAUL GARCIA, CHRISTOPHER WENTWORTH, Dept. of Physics, Doane College — Understanding diffusion in constrained geometries is of interest in a variety of contexts as varied as mass transport in disordered solids, such as a percolation cluster, or intercellular transport of water molecules in biological tissue. In this investigation we explore diffusion in a very simple constrained geometry: a comb-like structure involving a one-dimensional backbone of lattice sites with regularly spaced teeth of fixed length. The model considered assumes a fixed concentration of diffusing particles can hop to nearest-neighbor sites only, and they do not interact with each other except that double occupancy is not allowed. The system is simulated using a Monte Carlo simulation procedure. The mean-square displacement of a tagged particle is calculated from the simulation as a function of time. The simulation shows normal diffusive behavior after a period of anomalous diffusion that increases as the tooth size increases.

1Support provided by the Doane College Undergraduate Research Program

P1.00019 Transport Properties of Nanostructures1, AMIR MAHARJAN, H.E. JACKSON, L.M. SMITH, A. KOGAN, University of Cincinnati, J.Y. RICE, Miami University, Oxford, OH, C. JAGADISH, Australian National University, C. JAGADISH COLLABORATION — The current-voltage (I-V) properties of an InP nanowire and a CdS nanosheet are studied. Back to back metal semiconductor metal contacts are modeled based on thermionic emission theory and field emission theory. These are used to explain the I-V characteristics of these nanostructures which enables measurement of the important intrinsic properties including donor density and electrical conductivity of nanostructures. Photolithography followed by lift-off is used to fabricate the Al/Ti contact pads across these nanostructures for transport measurements. Scanning photocurrent microscopy (SPCM) is used to see the variation of photocurrent along the nanostructure. The SPCM image shows that the peak photocurrent always appears at the reverse biased metal-semiconductor contact edge indicating strong localization of electric field which is also confirmed by numerical simulation.

1UC start-up funds, NSF Grant No 0804199, ECCS-0701703 and DMR 0806700.
P1.00020 Chemical C-V Measurements on ZnO, Sarah Jane Gabig, Gary Farlow, Wright State University — When metal/semiconductor Schottky barriers are not practical, an electrolyte/semiconductor interface can be used to make capacitance-voltage (C-V) measurements. The physics of such electrochemical C-V measurements will be described. Electrical properties of ZnO were measured by electrochemical C-V techniques and photovoltaic spectroscopy using an Accent 4400 Electrochemical CV system. Specifically, the electrical behavior of a 0.1 M ZnCl₂ electrolyte-ZnO interface has been investigated with attention to the electrolyte-ZnO interface’s C-V dependence on carrier frequency.

P1.00021 The Heat Bath Monte Carlo Algorithm for the Ising Model of Ferromagnetism, Christopher Lemon, Ronald Johns, Ohio Northern University — The mathematical theory of Markov chains is placed in the context of the Ising model of ferromagnetism, an important problem in statistical physics. Although not a Markov chain itself, the two-dimensional Ising model can be simulated with the heat bath algorithm, which treats the Ising model as a Markov Chain. A Matlab program and variations were written that use Monte Carlo simulation and the heat bath algorithm to compute quantities arising in the Ising model. Results from this method were then compared to those derived from the mathematical definition of the Ising model. Based on the agreement of results, it can be concluded that the heat bath Markov Chain method is a convenient and valid method to simulate the two-dimensional Ising model.

P1.00022 Preparation and Characterization of Electrospun Alumina Nanofibers, Marie J. Pinti, Stephen N. Tackacacas, Nenad Stoiljkovic, Department of Physics, John Carroll University, John P. O’Brien, Anna Piscchera, Matthew P. Espe, Department of Chemistry, Knighnt Chemical Laboratories, The University of Akron — Alumina nanofibers are promising materials for use in high-temperature applications since they are chemically inert up to very high temperatures. Applications include use as catalyst support in high-temperature chemical reactions, fire protection materials, and as a high-temperature insulator. Electrospinning is a relatively simple and inexpensive method for obtaining nanometer-size fibers and has become a popular technique for producing metal-oxide nanofibers in recent years. The electrospinning mixture for the production of alumina nanofibers typically contains aluminum acetate stabilized with boric acid as the alumina precursor, but the observed presence of boron and sodium on the surface of these nanofibers may affect their use as catalytic supports. We have produced alumina nanofibers from an aluminum reagent devoid of the boric acid stabilizer and calcined the fibers at different temperatures to produce nanofibers with different phases of alumina. Characterization of the fibers by TGA, FE-SEM equipped with the XEDS, powder XRD, DRIFTs, and SSNMR methods to determine the fate of the precursors, fiber morphology and the composition and structure of the calcined alumina nanofibers.

P1.00023 XRD and DRIFTS study of Titania/Zinc Oxide Nanofibers, Stephen N. Tackacacas, Marie J. Pinti, Nenad Stoiljkovic, Physics Department, John Carroll University, Adria F. Lotus, George G. Chase, Department of Chemical and Biomolecular Engineering, The University of Akron — Titania nanofibers are very promising materials for high-temperature applications, and in recent years, electrospinning has been typically used for their production. With the objective of controlling the properties of the formed nanofibers, titania nanofibers doped with zinc oxide were annealed at different temperatures. Characterization of these fibers involved the use of TGA, powder XRD, SEM and DRIFTS methods; allowing a better understanding of formation of these materials, and determination of their structure and composition.

P1.00024 Evidence for Multiple Negative-Parity Band Structure in $^{71}$Se, N.R. Baker, Ohio Wesleyan University, R.A. Kaye, S.R. Arora, Ohio Wesleyan University, John Bruckman, Monmouth College, S.L. Tabor, T.A. Hinners, C.R. Hoffman, S. Lee, Florida State University, J. Doring, BFS, Germany — The negative-parity bands of $^{69}$Se and $^{71}$Se indicate a stark contrast between strong single-particle ($^{69}$Se) and collective ($^{71}$Se) behavior over a wide range of spins. However, only one negative-parity band has been observed so far in $^{71}$Se, making it difficult to see whether it lies between these two very different cases. Thus, the goal of the present work was to extend the level scheme of $^{71}$Se as much as possible, with an emphasis on finding new negative-parity states. $^{71}$Se nuclei were produced at high spin following the 80-MeV $^{54}$Fe($^{23}$Na, $\alpha$pn) reaction at Florida State University. $\gamma - \gamma$ coincidences were measured using an array of 10 Compton-suppressed Ge detectors which included three Clover detectors. From the coincidence relationships, new states were found that formed candidates for perhaps two new negative-parity bands. Cranked-shell model calculations indicate that one new band is associated with rigid-body rotation at high spin.

P1.00025 Power-scalable, polarization-stable, dual-colour DFB fibre laser system for CW terahertz imaging, Finn Eichhorn, DTU Fotonik, Department of Photonics Engineering, Technical University of Denmark, Jens Engholm Pedersen, Koheras A/S, Denmark, Peter Udd Jepsen, DTU Fotonik, Department of Photonics Engineering, Technical University of Denmark — Imaging with electromagnetic radiation in the terahertz (THz) range has received a large amount of attention during recent years. THz imaging systems have diverse potential application areas such as security screening, medical diagnostics and non-destructive testing. We will discuss a power-scalable, dual-colour, polarization-maintained distributed feedback (DFB) fibre laser system with an inherent narrow linewidth from the DFB fibre laser oscillators. The laser system can be used as source in CW THz systems employing photomixing (optical heterodyning) for generation and detection and is an alternative to pulsed THz systems using femtosecond lasers. The laser system generates output powers up to several hundred mW, has a 25 kHz linewidth and a polarization extinction ratio of better than 20 dB. Since the output power reaches the Watt-level, the laser system is a suitable candidate for future multi-channel THz imaging systems.

P1.00026 Improving Corrosion Diagnostics with Terahertz Sensors, 1 Stanley Smith, Beaver Creek High School, Lindsey Owens, Douglas Petkie, Jason Deibel, Wright State University, Department of Physics, Wright State University Collaboration, Institute for the Development and Commercialization of Advanced Sensor Technology Collaboration, Beaver Creek High School Collaboration — The objective of this project is to characterize metal samples using terahertz imaging to determine whether terahertz frequency radiation can detect the difference between corroded and clean metal including samples obscured with coatings of paint. A terahertz imaging system was used at incident angles of 45 and 90 degree to characterize the metal samples. Multiple imaging techniques were utilized such as time-domain amplitude imaging, single frequency amplitude imaging, and time-domain reflectometry. The images indicate that terahertz imaging does detect a noticeable difference between corroded and clean metal including measurements performed on painted samples. 1The authors would like to acknowledge Adam Cooney at AFRL-RXB for providing samples and the following organizations for funding support: IDCAST, WSU CoSM, and the WSU Office of RSP.

P1.00027 Spicing up Science: Mini Undergraduate Research Projects in Physics and Chemistry, George Devendorf, Indiana Academy, Ball State University — Individual student research projects are often small pieces of a larger research program and may or may not provide an interesting and satisfying research experience for a student researcher who only is engaged in the project for a limited time. This researcher describes a variety of research activities conducted with advanced high school students in a high school setting. These research projects are limited by the academic experience of the student, facilities and resources and available time. Such limitations however, have shaped some of the research projects into “mini-projects” that form interesting scientific questions which can be addressed within a semester or yearlong project. Several of these research ideas have been inspired from teaching introductory courses and though they may not further a continuing research program or spawn significant publications, they do provide an avenue for teaching and inspiring scientific inquiry in the minds of young potential scientists.
P1.00028 Kinematics from footprints: Analysis of a possible dinosaur predation event in the Cretaceous Era, SCOTT LEE, University of Toledo — Motivation is enhanced by challenging students with interesting and open-ended questions. In this talk, a methodology for studying the locomotion of extinct animals based on their footprint track-ways is developed and applied to a possible predation event recorded in a Cretaceous Era deposit. Students usually love learning about dinosaurs, an unexpected treat in a physics class. This example can be used in the classroom to help build critical thinking skills as the students decide whether the evidence supports a predation scenario or not.


P1.00029 Discovering and Understanding Misconceptions in Fifth grade Academic Content Standards, ADAM HICKS, JENNIFER BLUE, Miami University — Misconceptions are known to be prevalent among students, especially younger students. However, misconceptions can become engrained in the scientific thought process and linger throughout a person’s life. This study examines the results on test questions regarding the physical and space science from the fifth grade Ohio Academic Content Standards (Ohio Department of Education, 2003). Tests have been developed to evaluate the Southwest Ohio Science Institutes (http://www.units.muohio.edu/sosi), which teach content knowledge to teachers. These tests have been given to fifth grade teachers who participated in the institutes and to their students. The same questions were also given to university students. Eventually, the results from all three groups will be compared to find the persistence of misconceptions. This presentation will focus on the results from the university students.

P1.00030 Observation of quasi-periodic route to chaos in driven dusty plasma, W.L. THEISEN, T.E. SHERIDAN, Ohio Northern University — Chaotic dynamics have previously been observed in a driven dusty plasma with three particles [T. E. Sheridan, Phys. Plasmas 12, 080701 (2005)] due to a resonance overlap between the center-of-mass and breathing modes. In the present work, the transition to chaos in this system is characterized as a function of driving amplitude for two different driving frequencies. In the first case, the driving frequency is matched to the frequency minimum of the Arnold tongue, while in the second case, the driving frequency is slightly above this value. Dynamics are characterized by the power spectrum, Lyapunov exponent, and correlation dimension, as a function of driving amplitude. For the higher driving frequency we observe asymmetric spectral sidebands at intermediate driving amplitudes, a clear indication of quasi-periodic dynamics. For large driving amplitudes the dynamics become chaotic.

P1.00031 Sheath area for large planar Langmuir probes, T.E. SHERIDAN, Ohio Northern University — Electrostatic (i.e., Langmuir) probes made of thin, circular disks are often used to determine plasma parameters (e.g., electron temperature and density) by analyzing the probe’s current-voltage characteristics. A probe biased below the plasma potential (i.e., the ion saturation regime) attracts positive ions and repels electrons, leading to the formation of a cathodic sheath around the probe. The probe’s effective collecting area is determined by the sheath area, which, for a given probe radius, depends on the probe’s bias. The structure of this sheath is calculated using a particle-in-cell (PIC) code with kinetic ions and Boltzmann electrons by allowing a pulsed sheath to relax to a steady-state configuration. The Bohm criterion is used to define the sheath edge, which is taken to be the surface on which the average ion velocity equals the ion acoustic speed. The sheath area is calculated for probe radii from 50 to 200 times the electron Debye length biased from -5 to -50 times the electron temperature. The sheath area is found to have a power law dependence on both probe bias and probe radius.

P1.00032 Laue X-Ray spectrograph for the 200-TW Trident Laser, NALIN VUTISALCHAVAKUL, Ohio Wesleyan University, JAMES COBBLE, JONATHAN WÖRKMAN, KIRK FLIPPO, DAVID MONTGOMERY, SANDRINE GAILLARD, Los Alamos National Laboratory — With the 200-TW laser at the Trident Laser Facility, experiments on x-ray backlighting were performed. The sub-ps short pulse laser with energy up to 100 J can be shot on targets with different atomic number. The focused laser beam has intensities up to $10^{21} \text{W/cm}^2$. The high energy laser interacted with the targets, producing X-rays due to K-shell emission. Among other diagnostic devices, a Laue X-ray spectrograph was used to record the x-ray spectrum, which showed emission lines and bremsstrahlung radiation. The Laue spectrograph uses a LiF(200) crystal to disperse the x-ray spectra with a bandpass of 17-70 keV. The spectra were recorded using Fuji image plates. The Laue instrument was designed to include a tungsten shield in the front, a magnetic trap, and a light trap to reduce background noise. Kα lines of Mo, Ag, and Sn were observed.

2 This research project is funded by the United States Department of Energy.

P1.00033 Measurements of the Non-Linear Coupling of Plasma Waves, E.K. SNIPES, Wittenberg University, J. MCCLENAGHAN, A.J. NOBLE, A.A. KABANTSEV, C.F. DRISCOLL, UCSD — A separatrix is created in a pure electron plasma column by applying a theta-symmetric wall voltage. This “squeeze” voltage traps less energetic electrons in either end and allows more energetic electrons to pass through. These trapped particles enable the novel Trapped Particle Diocotron Mode (TPDM). We excite an ordinary $m = 2$ diocotron mode at frequency $f_2$ to amplitude $A_2$ and observe the decay into the $m = 1$ TPDM at $f_1 = f_2/2$. The exponential growth rate, $\Gamma$, of the TPDM is obtained as a function of the amplitude $A_2$ as well as a function of the “squeeze” voltage which determines the frequency mismatch $\delta f = f_2/2 - f_1$. We calibrate the amplitudes of the modes in terms of the received wall voltages, and obtain a quantitative value of the non-linear coupling coefficient, $V$. These results at $B = 280$ G will be compared to recent results from a separate apparatus at $B > 2000$ G.

2 Supported by NSF/REU PHY-0552402 and NSF PHY-0354979.

P1.00034 Modeling Rotation of H in Cu-H Defect Complex in ZnO, ANDREW MAGYAR, Ohio Northern University — The rotational motion of the bond-centered H or D atom in an isolated Cu-H defect complex in the ZnO crystal lattice is modeled under uniaxial stress. The uniaxial stress is applied along the c-axis of the crystal and causes an absorption line at 3229 cm$^{-1}$. The exponential growth rate, $\Gamma$, of the TPDM is obtained as a function of the amplitude $A_2$ as well as a function of the “squeeze” voltage which determines the frequency mismatch $\delta f = f_2/2 - f_1$. We calibrate the amplitudes of the modes in terms of the received wall voltages, and obtain a quantitative value of the non-linear coupling coefficient, $V$. These results at $B = 280$ G will be compared to recent results from a separate apparatus at $B > 2000$ G.

P1.00035 Capacitance-Voltage Properties of AlGaN Schottky Devices, A. DI MASCIO, M. AHOJJA, S. ELHAMRI, R. BERNER, Department of Physics, University of Dayton, OH — Electrical properties of Si doped AlGaN films, grown by radio-frequency plasma assisted molecular beam epitaxy, are investigated using variable frequency capacitance-voltage as a function of temperature. In particular, a comprehensive investigation of the properties of Ni/Au Schottky contacts as a function of temperature and frequency will be reported.
P1.00036 On the Doppler Deviation between the Temperatures of the Microwave Background Obtained by COBE. DMITRI RABOUNSKI — The COBE satellite, located in a 900 km orbit, gives two temperatures of the Penzias-Wilson microwave background: 2.730±0.001 K measured by the absolute spectrophotometer and 2.717±0.003 K calculated from the temperature of the dipole component (the 1st derivative of the monopole) measured by the differential radiometer. This deviation, 0.013 K, is 10 times exceeding the measurement precision. If, according to the experimental analysis by Robitaille (Prog. Phys., 2007, v.1, 3, 19), the microwave background is generated by the oceans of the Earth, this deviation meets a clear theoretical explanation by Rabounski (Prog. Phys., 2007, v.1, 24) as the Doppler effect of the dipole anisotropy due to the motion of the monopole in common with the source, the Earth, relative to the intergalactic foreground at 365 km/sec. According to this theory, there is no the monopole component at the L2 point (1.5 mln km from the Earth, the position of the WMAP and PLANCK satellites) due to its decrease with altitude. In contrast to WMAP, whose differential components target the dipole anisotropy, PLANCK will have on board absolute instruments and be able to give a proof to this theory.

P1.00037 Building New Dynamic Light Scattering Spectroscopy System. MAXWELL ORSENO, KIRIL STRELETZKY. Cleveland State University — Our goal is to construct a high resolution, versatile Light Scattering Spectroscopy Setup. When complete, this system will allow measurements with Dynamic Light Scattering and Static Light Scattering techniques, with polarized and depolarized light, several different laser wavelengths, and a wide range of scattering angles and temperatures. The first task was to get the Ar-ion laser operational. A water cooling system for the laser was developed and installed. Laser bases for the Ar-ion laser as well as a He-Ne laser were designed and machined. A system of mirrors that allows for a quick change from one laser to the other was added. The Ar-ion laser itself was tuned for optimal output. The light scattering spectroscopy system was aligned and test experiments were run on it. The data, after collected and analyzed, was compared with the data on existing Dynamic Light Scattering setup. The new results demonstrate that both polarized and depolarized Dynamic Light Scattering experiments of high accuracy can be successfully performed at several different laser wavelengths and a range of scattering angles using the new Light Scattering Setup. Careful tests of Static Light Scattering on the new system are still needed to be performed.

P1.00038 Experimental progress toward creating optical crystals of ultracold atoms. NATHAN SOUTHER, RICHARD WAGNER, MATTHEW BRIEL, SAMIR BALL, Department of Physics, Miami University — We propose an experiment to form an optical crystal using atoms that have been laser-cooled to temperatures of a few microKelvin. First we create an optical lattice — an array of periodic potential wells, half an optical wavelength apart, formed by intersecting laser beams, with about one well out of hundred occupied by an atom. Next, we use another beam to superpose a long-range periodicity on the lattice — causing wells located every few wavelengths apart to be deepest. This creates what is called a superlattice, where the atoms eventually collect in the lowest wells thus creating a long-range "crystal." This is called a crystal, not a lattice, because the probability of an atom occupying the periodic array of deepest wells is unity. Such optical crystals may have far-reaching implications for nanolithography and quantum computing.

P1.00039 Detection and Characterization of a Laser Induced Plasma. MICHAEL DEXTER, MATTHEW BOHN, Air Force Institute of Technology. — A plasma is generated and detected in ambient air using a 50 femtosecond, amplified Ti:sapphire laser at 800 nm and its second-harmonic at 400 nm. The plasma is monitored as a function of laser polarization and amplitude using an ultrasonic sound detector. The second-harmonic is generated in a BBO crystal located in a 1:1 telescope. The group delay of the second harmonic through the collimating lens of the telescope will be calculated and the resulting experimental complication requiring the separation of the fundamental and second-harmonic will be discussed. The goal of the experiment is to generate terahertz via the mixing of the second-harmonic and the fundamental in the plasma. The mechanism for terahertz generation in a plasma will be introduced as resulting from either a transient current or via four-wave mixing. The terahertz radiation can be detected using either the electro-optic method or a liquid He cooled silicon bolometer. The prospects of using this terahertz generation method in a two color femtosecond enhancement cavity will be discussed.

P1.00040 Solvent Effect on Linear Photophysical Properties of a Two Photon Absorbing Dye. JENNIFER MONAHAN, AFRL/RX, SOCHE, WSU-Chemistry Dept. — We undertook an investigation in order to determine the effect of solvent on the linear photophysical properties of a two photon absorbing dye. A solvent study was undertaken in which AF240 was investigated in order to determine the effect of solvent on the linear photophysical properties of this dye. A solvent study was undertaken in which AF240 was investigated in order to determine the effect of solvent on the linear photophysical properties of this dye. The solvent used in these experiments was water and ethanol, and the second-harmonic at 400 nm. The plasma is monitored as a function of laser polarization and amplitude using an ultrasound detector. The second-harmonic is generated in a BBO crystal located in a 1:1 telescope. The group delay of the second harmonic through the collimating lens of the telescope will be calculated and the resulting experimental complication requiring the separation of the fundamental and second-harmonic will be discussed. The goal of the experiment is to generate terahertz via the mixing of the second-harmonic and the fundamental in the plasma. The mechanism for terahertz generation in a plasma will be introduced as resulting from either a transient current or via four-wave mixing. The terahertz radiation can be detected using either the electro-optic method or a liquid He cooled silicon bolometer. The prospects of using this terahertz generation method in a two color femtosecond enhancement cavity will be discussed.

P1.00041 Laser-Excited Fluorescence Spectroscopy of Br2: NIR Transitions to High Vibrational Levels in the (1Σ+g′) State. DAVID DOLSON, DAVID POSTELL1, Department of Chemistry, Wright State University, Dayton, OH 45435, GLEN PERRAM, Department of Engineering Physics, Air Force Institute of Technology, Wright-Patterson AFB, OH 45433 — The B(2Πu′,v″) – X(1Σ+g′) laser-excited fluorescence spectrum of Br2 was recorded with rotational resolution in the visible and near infrared (NIR) spectral regions to 1400 nm. The line-narrowed (0.2 cm⁻¹) output of a 532 nm pulsed Nd:YAG laser was used to excite eight fluorescence progressions in a natural abundance sample. Six of the excitation transitions occur in the 79,81Br2 isotopomer and one each in the 79Br2 and 81Br2 isotopomers. NIR fluorescence transitions from the 25 ≤ v′ < 33 laser-excited levels to the 28 ≤ v″ ≤ 44 vibrational levels in the ground state were observed between 950 nm and 1400 nm. The 97 lines from this NIR data set were combined with 6300 lines calculated with the data of Focsca et al [J. Mol. Spectrosc. 200, 104-119 (2000)] to derive a set of Dunham coefficients for the ground state. An X(1Σ+g′) state KKR potential curve also was constructed for vibrational levels, v″ = 0 – 44, which extends three quarters of the way to the dissociation limit.

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Friday, October 10, 2008 8:00PM - 9:00PM —
Session B1 Public Lecture Oelman Hall 109

8:00PM B1.00001 Improbable Research and the Ig Nobel Prizes. MARC ABRAHAMS, Improbable Research — The Ig Nobel Prizes honor achievements that first make people laugh, then make them think. Marc Abrahams, father of the Ig Nobel Prize ceremony and editor of the magazine Annals of Improbable Research, will show us some of the most outstanding Ig Nobel winners. He will also discuss why Ohio has been such a good producer of Ig Nobel Prize winners, and of improbable research.
GORDON AUBRECHT, Ohio State University at Marion — We attempted to determine what topics seem hardest for students taking the Physics by Inquiry course. We characterized student performance using a formative assessment tool called ‘Properties of Matter’. We found that the topics of light and waves, as well as mechanics, were among the hardest for students. This suggests that more focused attention on these areas is needed to improve student understanding.

Wire Pairs

NICHOLAS SCHROEDER, FIN EICHORN, JASON DEIBEL, Wright State University — The objective of this project is to capture the spectroscopic signature and temperature of combustion process as a function of position using terahertz (THz) time-domain spectroscopy and imaging. The development of a system that can monitor the temperature of an exhaust plume and its chemical make-up as a function of position would be of immeasurable value to the further development of jet engines and their mid-life diagnostics. Current techniques available require different set-ups for each measurement, position and chemical. Our approach to tomographic reconstruction consists of utilizing 8 separate THz transmitter-receiver pairs arranged around the object, allowing all of the tomographic slices to be taken at the same instant. We will present preliminary data demonstrating THz tomographic imaging of solid objects and calibration of spectroscopic and thermal measurement capabilities by THz characterization of water vapors and flames. We will further show ongoing work to produce a THz tomographic reconstruction of a simple flame.

Terahertz spectroscopy of gas phase molecules for chemical physics applications

DOUGLAS T. PETKIE, Wright State University — By far the most successful chemical physics application in the terahertz region has been high resolution spectroscopy of gas phase molecules. Laboratory investigations probe the molecular structure and intramolecular forces of a molecule and make possible the expansive databases for monitoring chemical species in the upper atmosphere and identification of molecules in the interstellar medium. Translating these technologies to terrestrial applications can be challenging due to broadband line widths at atmospheric pressures. An overview of laboratory and remote sensing applications will be presented as well as the challenges of terrestrial remote sensing.

Nondestructive materials characterization using sub-millimeter wave imaging

IZAAK KEMP, DOUGLAS T. PETKIE, Wright State University — A sub-millimeter continuous wave system can be used to image corrosion pitting and structural defects in common aircraft materials such as aluminum 2024. In order to avoid failure of components during operation, many aircraft parts are replaced earlier than necessary leading to higher costs that could be reduced if the degree of damage in the component material could be determined non-destructively. Sub-millimeter wave systems are ideally suited for this purpose because of their ability to penetrate through substances such as paint, oil, and epoxy commonly found on the surfaces of aircraft. We will discuss the system we are developing and several set of results.

Non-Destructive Corrosion Detection Using Terahertz Time-Domain Spectroscopy and Imaging

LINDSAY OWENS, STANLEY SMITH, Student, DOUG PETKIE, JASON DEIBEL, Professor, WRIGHT STATE UNIVERSITY TEAM, BEAVERCREEK HIGH SCHOOL TEAM, AFRL MATERIALS DIRECTORY TEAM — The objective of this project is to detect corrosion of manufactured metal underneath a paint. The system used in this research is a commercial terahertz time-domain spectroscopy and imaging system. THz signals are generated and detected using optical excitation of biased semiconductor antennas with 100 femtosecond pulses from an 800 nm laser. Spectral images were of metal samples were taken at frequencies between 100 GHz and 1 THz using a variety of imaging modalities in both transmission and reflection. Preliminary imaging data shows a clear distinction between corroded and clean metal concealed underneath a coat of paint.

FEM Simulation of a Terahertz Metamaterial using Short/Long Metal Wire Pairs

ZACH GAULT, SCOTT EILERMAN, JASON DEIBEL, Wright State University, WRIGHT STATE UNIVERSITY COLLABORATION, IDCAST COLLABORATION — The goal of our work is to develop a successful metamaterial model with an intended negative index of refraction using a simple metal structure on a dielectric substrate. We have developed a structure consisting of short and long straight-wire pairs with a resonance at 0.1 THz. In order to optimize the design parameters of the metamaterial device, we use finite element method (FEM) simulations. We will show how the frequency-dependent transmission data is evaluated to determine the device’s effective index of refraction, as well as discuss efforts to fabricate a THz metamaterial device and characterize it using terahertz time-domain spectroscopy.

The authors would like to acknowledge the following funding sources: IDCAST, WSU CoSM and WSU Office of RSP.
8:24AM C2.00003 Changing student's attitudes about teaching in a science course for teachers, TODD SMITH, MARY KAY KELLY, The University of Dayton, BETH BASISTA, Wright State University — Teacher education programs generally have different courses designed to give pre-service teachers multiple opportunities to develop as teachers. Science content courses, general methods courses, and field experiences help the pre-service teacher to begin to develop pedagogical content knowledge (PCK). However, research has established that one of the difficulties for pre-service science teachers is the disconnect between how they have learned their science content and how they are expected to teach that science content to K-12 students. Science content courses for pre-service teachers can be enhanced when content-specific best practices are incorporated, modeled, and made explicit. We have studied the effect of modeling content-specific best practices in a physics content course at The University of Dayton by assessing the students’ content knowledge and attitudes towards teaching both before and after the course. The results of our study will be presented in this talk.

8:36AM C2.00004 Hosting a Successful Science Fair to Boost Interest in Science, JAMES SULLIVAN, THOMAS CRUSE, University of Cincinnati — Science fairs are a popular way for junior and senior high school students (grades 7 through 12) to display science and engineering projects and participate in a competition for prizes and honors. In the state of Ohio students can advance through their school fairs to district science fairs and then on to the State Science Day in early May. The University of Cincinnati (UC) has hosted one of the Ohio district science fairs since 2005 - the official name is the UC Science and Engineering Expo (UCSEE). The University hosts between 300 and 400 student projects at this event. The day itself includes the training of the 200+ judges, the actual judging, activities for the students’ family members, and student competitions. In addition, we have used this event to involve the community through local community groups and state sponsorship with a guest speaker and an awards ceremony. The students compete for prizes and scholarships worth approximately $50k and over 100 of the UCSEE projects typically advance to participate in State Science Day. Additionally some top projects from the UCSEE are also sent directly to the International Science and Engineering Fair (ISEF). The authors have been heavily involved in the planning, organization and production of the UCSEE since UC began offering it in 2005. Much of the planning and background work, as well as memories, from this major project will be discussed in this presentation.

8:48AM C2.00005 Working to have an IMPACT1, GORDON AUBRECHT, Ohio State University at Marion — In 2004-2005. I was part of a team that won a Department of Education grant, known as IMPACT. We worked with K-12 teachers in Marion and Newark, helping them rethink how they were teaching, helping them ask more (and better) questions. Some of the teachers were in the middle school in Marion, Ohio. They contacted the administration of the City Schools and suggested that I be involved in improving science scores at the middle school level. We submitted a seed grant proposal to the Ohio Department of Education that was funded. We had teacher buy-in; the union agreed and each teacher agreed to be part of the program. We submitted a full proposal, with the title “Systemic Change Through Embedded Professional Development at a STEM+C Middle School (IMPACT II),” which was funded. We envision our program to involve teachers in hands-on activities and questioning. This talk will present more details of the program currently being implemented at Grant Middle School.

Saturday, October 11, 2008 8:00AM - 9:24AM — Session C3 Chemical Physics — Fawcett Hall 206

8:00AM C3.00001 System-averaged exchange and correlation holes in second-row atoms, ANTONIO CANCIO, Ball State University — Recent work is presented on the theoretical calculation of system-averaged exchange and correlation holes (intracules) for a pseudopotential model of the valence shell of second-row atoms. Exchange holes are obtained from numerical fourier transform methods and correlation holes from variational quantum Monte Carlo calculations using the method of correlated estimates. We observe approximate scaling behavior in both exchange and correlation, following the known scaling of the valence density across the row. The holes are compared to density-functional models including LDA, GGA and meta-GGA approaches. Particular attention is paid to self interaction (SI) error; we find that a sizeable error occurs in the same-spin channel of the correlation hole which persists for the LDA and GGA even after standard SI corrections are applied. A simple SI correction that eliminates this error will be discussed.

8:12AM C3.00002 The Adiabatic-to-Diabatic Mixing Angle for B + H₂ Potential Energy Surfaces, MATTHEW GARVIN, DAVID WEEKS, Department of Engineering Physics, Air Force Institute of Technology, Wright-Patterson AFB, Ohio 45433 — The 1A′, 2A′, and 1A″ adiabatic potential energy surfaces and associated nonadiabatic coupling terms are calculated at the state-averaged MCSCF/CI level. A line integral through the nonadiabatic coupling terms is used to calculate the adiabatic-to-diabatic mixing angle required to transform from the 1A′ and 2A′ adiabatic basis to a corresponding diabatic basis. When all nonadiabatic coupling terms between all electronic states are considered, the line integral will transform one diabatic state at a time. If some of the diabatic states are identical or equivalent, we consider only nonadiabatic coupling terms between the 1A′, 2A′ and 2A″ states and the line integral is therefore path dependent. The path dependence of the line integral is then used to characterize the error introduced by employing a truncated set of adiabatic states. A method for reducing the effect of this error through the use of symmetry derived boundary conditions is discussed.

8:24AM C3.00003 Surface effect on the medium-range structure of colloidal and mesoporous silica1, GANG CHEN, KUANGMIN LI, CONGSHANG WAN, Ohio University, DEPARTMENT OF PHYSICS AND ASTRONOMY TEAM — Glasses synthesized by the conventional melt-quenching method and by the sol-gel method do not have exactly the same structure. To understand the medium-range structure of sol-gel derived silica glasses, we have conducted small-angle and wide-angle x-ray scattering experiments on colloidal and mesoporous silica. Effects of particle/pore size and thermal treatment on the first sharp diffraction peak (FSDP) of the silica have been studied. It is found that the FSDP of colloidal silica (1A′ and 2A′) and mesoporous silica (1A″ and 2A″) differs. The FSDP of colloidal silica depends on the silica size, and that of mesoporous silica is independent of pore size. The FSDP of mesoporous silica is high at high temperature and can shrink in the pore width and change in the FSDD. Our study suggests a close relationship between the surface properties and the medium-range structure of sol-gel derived silica glasses.

1GC acknowledges Ohio University Startup Fund for supporting this work.

8:36AM C3.00004 Nuclear Magnetic Conduits, RICH DESANTIS, APS — Point charges are not conduits of magnetism. Vacuum gaps between charges prevent superconductivity. Magnetism occurs w/o charge velocity. A changing magnetic field can add magnetism, w/o magnetism’s centripetal force adding speed. Voltage is not charge repulsion energy. Passing electrons through a stationary electron’s field cannot reduce its field. Passing the external electrons through a charged capacitor’s field discharges the capacitor. Chemical bonds extend between atoms. A superconductive magnet contains a superconductive molecule, the length of its wire. Superconductivity dictates that chemical bonding material is non-vacuum and non-point charge. Its unit is an electron/proton fusion called an ABION. Unpaired abions attract all other unpaired abions within or between atoms. Paired abions have had reduced attraction for other abions. Helium is inert because its abions are paired. A lithium atom includes an unpaired abion. Superconductive abions are nuclear magnetic conduits. Equality of transference numbers in electrochemistry is evidence of conduits. In fuel cells and semiconductors, paired voltage-induced redox reactions convert lines of abions into conduits. This temporarily converts bulk insulators to conductors.
8:48AM C3.00005 Investigating the Diffusive Behavior of HPC with DLS and FPR, RYAN MCDONOUGH, KIRIL STRELETZKY, CSU, PAUL RUSSO, LSU — Hydroxypolycellulose (HPC) polymer chains were dissolved in aqueous solution in order to explore their diffusive qualities. Two fundamentally different methods: FPR (Fluorescence Photo-bleaching and Recovery) and DLS (Dynamic Light Scattering) were employed to study the structure and dynamics of HPC chains. FPR requires polymer to be chemically tagged by fluorescent molecules. FPR captures diffusion by establishing a photo-bleached boundary, observing only tagged particles diffusing back into the bleached area, yielding a contrast decay function. DLS auto-correlates scattered light intensity from particles, calculating a decay function which yields information about the self diffusion of particles at chemical equilibrium. An Inverse Laplace Transform Algorithm (CONTIN) and stretch exponential line shape analysis (LSA) quantitatively decomposed spectral decays into diffusion processes or modes. The LSA and CONTIN analysis on the same FPR decay spectra resulted in roughly similar modal distribution and mode intensity results. The modal distributions for FPR and DLS spectra on the same sample have shown consistent dissimilarities which may indicate a comparative limitation and/or sensitivity to a particular range of diffusive speeds or processes. The tag and/or tagging process appear to alter samples in a way that is quantifiable and consistent. The nature of diffusive processes in HPC appears to be complex, but analysis reveals a reproducible picture.

9:00AM C3.00006 Production of Singlet Oxygen within a Flow Discharge, MATTHEW LANGE, GREG PITZ, GLEN PERRAM, AFIT — The Airborne laser program is an Air Force sponsored program to place a laser on the battle field for use as a tactical weapon. The chemical oxygen iodine laser offers the powers necessary for this weapons application, but it requires significant logistical support. The goal of this current research program is to demonstrate an oxygen-iodine laser with electrical discharge production of singlet oxygen. Optical diagnostics have been applied to microwave and radio frequency discharges within a pure oxygen flow. The O$_2$(a) emissions within a discharge are complicated by atomic oxygen emission requiring care in determining gas concentrations from optically measured emissions. Thermal effects also complicate optical emissions. The inclusion of vibrationally excited oxygen as a quencher of the O$_2$(a) state appears to be the limiting rate for production of O$_2$(a) within the electric discharge conditions studied in this research.

9:12AM C3.00007 Temporal Evolution of Arc Emission From Laser REMPI Triggering of Air Spark Gap, JARED MILES, STEVEN ADAMS, Propulsion Directorate, Air Force Research Laboratory, WPAFB/WSU COLLABORATION — A laser-triggering scheme for air spark gap switches was conceived and experimental data presented. The laser-induced breakdown was analyzed to investigate arc formation. The scheme utilized a pulsed ultraviolet laser to generate resonant enhanced multi-photon ionization (REMPI) within the atmospheric air medium of a spark gap switch. With an applied voltage below the self-breakdown level, the laser-induced pre-ionization initiated avalanche breakdown within the gap and the subsequent triggering of the switch. The pre-ionization was made possible by utilizing resonant 2-photon absorption, exciting O(3Π$_g^+$) to the O$_2$(C$^2Π_g$, v=2) state, followed by an ionization laser with added laser power. The focused laser beam created a pre-ionization channel within the gap establishing the arc path. The spectral and spatial distributions of the emission as a function of time were analyzed to help determine the mechanism for arc formation. Spectral images of the N$_2$(C$^2Π_u$ - B$^2Π_u$) bands indicated when direct electron impact was the dominant ionization, while N$^+$ atomic ion bands indicated that voltage collapse and thermal ionization was occurring.

Saturday, October 11, 2008 8:00AM - 9:24AM — Session C4 Astronomy and Nuclear Physics, Fawcett Hall 108

8:00AM C4.00001 A note on the quantum-tail effect on fusion reaction rate, ALEXANDER ZUBAREV, Purdue University — A study is made of the power-law tail effect in the quantum particle distribution over momentum on the nuclear fusion reactions. Our results [1] do not support the idea of averaging the fusion reaction cross-section over the momentum distribution, postulated and used in many publications.


8:12AM C4.00002 Track Reconstruction for the NIFFTE TPC, SARVAGYA SHARMA — The Global Nuclear Energy Partnership (GNEP) has funded the construction of a Time Projection Chamber (TPC) to be used for precision fission cross-section measurements through the Nuclear Energy Research Initiative (NERI). This poster will illustrate the status of algorithms intended for intelligent track finding and track fitting using raw data obtained TPC simulations. The track fitting effort in this experiment has borrowed a number of ideas from high-energy physics along with other pattern recognition techniques not previously affiliated with experimental physics. Two track-finding techniques have been investigated. The Hough Transform is a brute force attempt at finding tracks. The second paradigm for track reconstruction, Binary Space Partitioning (BSP) was found to be less computationally expensive than the Hough Transform. BSP has been borrowed from the field of computer animation and rendering. To determine track fit parameters, an iterative Kalman Filter has been implemented that allows multiple scattering and energy losses to be taken into account to obtain unbiased errors. Fitted tracks obtained from the Kalman Filter were used to generate the best kinematic fit for the vertex.

8:24AM C4.00003 Global Warming and the Microwave Background, PIERRE-MARIE ROBITAILLE, The Ohio State University — The energy balance of our planet is determined by the relationship between absorbed (solar) and emitted (earthly) radiation. In many models, the Earth’s radiation is derived by applying Stefan’s Law, at a given effective temperature, thereby treating the globe as a uniform blackbody source. However, the oceans cannot be treated as simple blackbody emitters. In fact, while water can provide strong emission bands in the IR, the spectrum is far from blackbody. This is particularly important in the microwave region where the oceans mimic a 3K blackbody source (the Penzias and Wilson signal). As a result, the oceans are poor emitters of radiation in this spectral range. Their inability to efficiently emit radiation results in substantial retention of thermal energy by the oceans.

8:36AM C4.00004 Galaxy Properties and Substructure in the Cluster Abell 160, CRAIG KOONTZ, JASON PINKNEY, Ohio Northern University — We continue development of a procedure for building a large catalog of cluster galaxies and their photometric properties, as measured with CCDs. Of the first case, Abell 160, is relatively nearby and we have already obtained spectroscopic redshifts for its brightest galaxies. We have mosaiced this cluster in R and V filters using a CCD imager on the 1.3-meter McGraw-Hill telescope. For each CCD frame we fit a WCS (world coordinate system), remove bright cosmic rays, and extract sources using “SExtractor.” We create software for merging source catalogs in such a way as to reject residual cosmic rays and other invalid sources, and to combine redundant measurements without double counting. The measured properties include magnitude, ellipticity, position angle, size, and color (V-R). We compare our data to those of the HST (Hubble Space Telescope) and SDSS (Sloan Digital Sky Survey) archives to examine the accuracy of our star/galaxy separation and our color measurements. For our substructure investigation, we drew several subsamples of galaxies based on stellar index, color (the color-magnitude relation), magnitude and velocity. The smallest subsample of spectroscopically confirmed members produces significant substructure signals from 1D (velocity) and 3D (x,y,velocity) diagnostics - a small, offset group may be the culprit. The 2D (x,y) diagnostics applied to the larger samples produce some significant statistics, the cause does not seem to be a large-scale merger, but perhaps several small groups. This is consistent with previous X-ray data showing X-ray emitting gas clumped around small groupings of galaxies.
8:48AM C4.00005 Improving the Archival Tools of NRAO, BRIAN L. SACASH, Ohio Northern University — In this project, we cataloged and scientifically characterized the data archives of two retired NRAO single dish telescopes and investigated the tools and techniques of archival research. The project involved creating a strategy for long-term data curation and access. We successfully updated the original data found by writing and using original software along with using software already in existence. Each of the files of all the archives had the proper metadata extracted in order to render the data searchable.

9:00AM C4.00006 Solar Cycle Characteristics Examined in Separate Hemispheres, JAMES GALLAGHER, Ohio Northern University — According to recent research results from solar dynamo models, the north and south hemispheres may evolve separately throughout the solar cycle. Using hemispheric sunspot area from the Royal Greenwich Observatory (RGO), we measured a phase lag between the north and south hemispheres for solar cycles 12-23, which ranged from 0-19 months. We examined the presence of a Gnevyshev gap to determine if the double-peak of any given solar cycle is caused by an averaging of two hemispheres that are out of phase. We confirmed previous findings that show the Gnevyshev gap to be a hemispheric phenomena and is not due to a superposition of sunspot indices from hemispheres slightly out of phase. We then measured the flux crossing the equator by examining Kitt Peak and SOLIS magnetograms for solar cycles 21-23 and found, on average, a surplus of northern hemispheric flux crossing during the mid-declining phase of each solar cycle.

9:12AM C4.00007 Nothing is Dark in the New Physics, JAMES BEICHLER — In previous APS meetings, I have presented a geometrical explanation of Dark Matter and Dark Energy that makes testable predictions and is thus completely falsifiable. The theory is based on a macroscopically extended fourth dimension of space, yielding a five-dimensional space-time structure. In this structure, the four-dimensional space-time of relativity is extrinsically curved in the higher spatial dimension. Dark Matter is curvature in the higher dimension that is not directly associated with local matter, but instead a result of the interaction between local matter or curvature and the global curvature due to all matter in the universe. Criticisms were leveled that the theory was not mathematical, i.e., there were no algebraic equations to describe the geometrical structure. However, a simple algebraic formula that describes and explains the geometry of the four-dimensional structure of space has since been derived. Although the algebraic formula appears to be Newtonian, it implies a five-dimensional unification of the gravitational and electromagnetic fields such as that accomplished by Kaluza in 1921 and extended by Einstein and his colleagues in the late 1930s. The new equation also shows how gravity can be quantized on the basis of relativity without hypothesizing the discrete nature of matter, i.e., the existence of specific ‘particles’ of gravity, inherent in quantum mechanics, the Standard Model and other quantum models.

Saturday, October 11, 2008 8:00AM - 9:12AM — Session C5 Atomic and Molecular Physics Fawcett Hall 218

8:00AM C5.00001 Infrared spectra of the detonation fireballs, BENJAMIN SCHOTT, KEVIN GROSS, GLEN PERRAM, Air Force Institute of Technology — A rapid scanning Fourier transform infrared spectrometer was used to observe the detonation of several novel munitions. The spectral signatures from different explosive compositions are discernable and may be exploited for event classification. A simplified radiative transfer model recently developed for the spectral interpretation of rapidly evolving battlespace combustion events has been extended and applied to the data from these new field tests. In particular, the fireball radius, temperature, soot combustion, and H2O and CO2 concentrations are determined as a function of time. The fireball radius increased from 0 to 8 meters in about 230 ms and decreased gradually over the following 1-3 s. The fireball temperature profile revealed a rapid jump to over 1800 Kelvin immediately upon detonation followed by a short oscillation as secondary combustion kinetics dominated and a longer temperature decay. Computational methods for fitting the radiative transfer model to the observed data will be discussed, with a particular emphasis on computational efficiency.

8:12AM C5.00002 Charge Transport in DNA with Five Base Pairs, SUNHEE LEE, ERIC HEDIN, YONG JOE, Ball State University — Recently, much interest has arisen in the process of charge transport through DNA due to its fundamental roles in biological processes and in possible novel molecular electronics. We investigate quantum mechanical electron transmission along the long axis of DNA having a one-dimensional tight-binding model. In this system, we consider a single central conduction channel in which individual sites represent a base-pair formed by either AT (TA) or GC (CG) pairs coupled via hydrogen bonds. The sites are linked by a hopping amplitude, or quantum overlap integral. The sugar-phosphate backbone and the hopping amplitude between each site of the base and the backbone are incorporated into an energy-dependent on-site potential in the main DNA site. For the sake of simplicity, a simple DNA molecule segment with five base pairs is studied, and the transmission for different values of on-site energy is calculated to determine the influence of mismatch (impurity) effects in the DNA sequence. Finally, we present results for the temperature dependence of the transmission, and the current-voltage characteristics in order to examine the extent and efficiency of charge migration. *One of the authors (E.R.H.) is partially supported by a grant from the Center for Energy Research, Education, and Service (CERES) at Ball State University.

8:24AM C5.00003 Hyper-spectral imaging of aircraft exhaust plumes, SPENCER BOWEN, KENNETH BRADLEY, KEVIN GROSS, GLEN PERRAM, MICHAEL MARCINIAK, Air Force Institute of Technology — An imaging Fourier-transform spectrometer has been used to determine low spatial resolution temperature and chemical species concentration distributions of aircraft jet engine exhaust plumes. An overview of the imaging Fourier transform spectrometer and the methodology of the project is presented. Results to date are shared and future work is discussed. Exhaust plume data from a Turbine Technologies, LTD, SR-30 turbojet engine at three engine settings was collected using a Telops Field-portable Imaging Radiometric Spectrometer Technology Mid-Wave Extended (FIRST-MWE). Although the plume exhibited high temporal frequency fluctuations, temporal averaging of hyper-spectral data-cubes produced steady-state distributions, which, when co-added and Fourier transformed, produced workable spectra. These spectra were then reduced using a simplified gaseous effluent model to fit forward-modeled spectra obtained from the Line-By-Line Radiative Transfer Model (LBLRTM) and the high-resolution transmission (HITRAN) molecular absorption database to determine approximate temperature and concentration distributions. It is theorized that further development of the physical model will produce better agreement between measured and modeled data.

8:36AM C5.00004 EIT Intensity Noise Spectroscopy, MICHAEL CRESCIMANNO, Youngstown State University, Dept. Physics and Astronomy, YANHONG XIAO, Harvard-Smithsonian Center for Astrophysics, MARIA BARYAKHTAR, Harvard University, MICHAEL HOHENSEE, Harvard University and the Harvard-Smithsonian Center for Astrophysics, DAVID PHILLIPS, Harvard-Smithsonian Center for Astrophysics, RON WALSWORTH, Harvard-Smithsonian Center for Astrophysics and Harvard University — Intensity noise correlations in coherently-prepared media can reveal underlying spectroscopic detail, such as power broadening-free resonances. We analyze recent experimental results using very simple theory: The intensity noise correlation spectra can be quantitatively understood entirely in terms of static ensemble averages of the medium’s state response. This is significantly simpler than stochastic integration of the Bloch equations, and leads to physical insights we apply to non-linear Faraday rotation and noise spectra in optically thick media.
8:48AM C5.00005 Intensity auto- and cross-correlations for a driven optical cavity coupled to a three-level atom1, PATRICK HEMPHILL, JAMES CLEMENS, Department of Physics, Miami University — We present two-time intensity auto- and cross-correlations for the light transmitted through a driven optical cavity coupled to a single three-level atom in the A configuration. The atomic transitions couple to two orthogonally polarized cavity field modes on resonance. One of the cavity modes is weakly driven by an external coherent field. We model this cavity quantum electrodynamics (QED) system using a quantum trajectory unraveling of the master equation based on direct photodetection of the transmitted light.

1Supported by Research Corporation under award number CC6822/6875

9:00AM C5.00006 Pressure broadening and shifting of the Cesium D1 and D2 lines by rare gases, DOUGLAS WERTEPNY, GREG PITZ, GLEN PERRAM, Air Force Institute of Technology — The Diode Pumped Alkali Laser (DPAL) offers a high power, electrically driven laser with excellent thermal management, lightweight packaging, and high brightness for tactical military applications. The concept of using a gas phase medium for the phasing of large diode arrays via a highly efficient, cyclical photon engine combines the best features of electrically driven lasers with the inherent thermal management advantages of a gas lasers. Matching the spectral bandwidth of the diode pump source with the atomic absorption profile is paramount and requires both the narrow banding of high power diode laser arrays and novel approaches to broadening the gas lineshape. In the present work, the rates for pressure broadening and line shifts are reported for both atomic and molecular collision partners using laser absorption and induced fluorescence techniques. The absolute absorption and stimulated emission cross-sections, including the effects of hyperfine splitting and pressure broadening at low to moderate pressures are computed and compared with experimental results.

Saturday, October 11, 2008 8:00AM - 9:12AM – Session C6 Condensed Matter Oelman Hall 302

8:00AM C6.00001 Temporal and spectral photoluminescence from HVPE grown GaAs, MATTHEW BOHN, Air Force Institute of Technology, WILLIAM GUINEY, Rose-Hulman Institute of Technology — Defects discovered in low temperature photoluminescence (PL) spectrum recorded from Hydride-Vapor Phase Epitaxial growth of GaAs were measured as a function of secondary HCl flow. An Argon ion laser illuminated the GaAs samples, which were held at 10 K using a liquid He cold finger in a cryogenic dewar. Transitions involving the point defects due to e-Si\textsubscript{4}, V\textsubscript{A}--Si\textsubscript{4}, and e-V\textsubscript{O}\textsubscript{C} are identified in the PL spectrum. The Si defects are plotted as a function of HCl secondary flow rate and carrier concentration. It is postulated that the Si defects are introduced into the growth due to the quartz tube used in the secondary flow. In addition, time resolved PL measurements were made using a femtosecond Ti:sapphire laser and a synchronized Hamamatsu streak camera capable of picosecond temporal resolution. The time resolved PL measurements of the samples substantiated the excellent quality of the crystalline growth.

8:12AM C6.00002 Diffusion in Polypropylenes: Effects of Stereochemistry and Polydispersity1, ERNST VON MEERWALL, NUMAN WAHEED, WAYNE MATTICE, University of Akron — We have performed pulsed-gradient diffusion (D) experiments at 180 deg. C and dynamic Monte-Carlo (MC) simulations to study the effect of stereochemoical composition of linear propylene (PP) melts. The coarse-grained simulations were based on the rotational isomeric state model and Lennard-Jones potentials. For the proton NMR diffusion measurements we obtained three PP specimens of differing molecular weight M and dispersity, with the probability of a meso diad Pm = 0.02 (syndiotactic), 0.23 (atactic), and 0.89 (nearly isotactic). Conversion between MC steps and real time was derived from experiment; no dependence on Pm is expected. Both simulation and M-scaled experiment found D at high Pm several times faster than at low Pm, but the constant-M simulations showed a maximum in D near Pm = 0.8 due to quenched randomness. To find the source of the remaining disagreement with experiment, new simulations tracked the samples’ mean D and polydispersity, but the disagreement actually increased. We suspect that the GPC determination of M and its distribution, based on linear polyethylene scaling, is strongly dependent on PP stereochemistry, producing the misleading result.

1Supported in part by NSF (DMR 04-55117).

8:24AM C6.00003 Calculating Young’s modulus for a carbon nanotube, FERAS ALZUBI, University of Central Florida, RONALD COSBY, Ball State University — Young’s modulus for an armchair single-wall carbon nanotube was calculated using an atomistic approach and density functional theory (DFT). Atomic forces and total energies for strained carbon nanotube segments were computed using Atomistix’s Virtual NanoLab (VNL) and ToolKit (ATK) software. For a maximum strain of one percent, elastic moduli were calculated using both force-strain and energy-strain approaches and density functional theory (DFT). Atomic forces and total energies for strained carbon nanotube segments were computed using Atomistix’s Virtual NanoLab (VNL) and ToolKit (ATK) software. For a maximum strain of one percent, elastic moduli were calculated using both force-strain and energy-strain approaches. The average values found for Young’s modulus were in the range 1.2 to 3.9 TPa depending on the cross-sectional area taken for the carbon nanotube, consideration of Poisson’s ratio, and the calculation method used. Three possible choices of cross-sectional area for the nanotube are discussed and parameter and convergence tests for the DFT computations are described.

8:36AM C6.00004 Multiconfiguration Hartree-Fock autoionization calculations near the 3p excitation edge of the transition metals, KOFI NUROH, Kent State University — We report electron-impact excitation relative scattering cross sections for the transition metals \textsuperscript{2}Ni near the 3p excitation edge. The first set of calculations is based on the theoretical model of random-phase approximation for core-electron scattering in solids in which only electrostatic interactions are taken into account. The second set of calculations is based on an analysis that hinges on the Bethe-Born approximation in which both electrostatic and magnetic interactions are incorporated. Both sets of calculations show trends in Z that are manifested in available measurements.

8:48AM C6.00005 Terrace Width Distributions in the Limit $\beta B / \beta A \to \infty$: Numerical Transfer Matrix Results, HOWARD RICHARDS, Marshall University — With a few physical and mathematical simplifications, the Terrace Width Distributions (TWDs) for a stepped crystal surface with typical step interactions have been shown to be Generalized Wigner Distributions (GWDs). This is true even when steps have different stiffnesses ($\beta A$ and $\beta B$) that alternate, as has been confirmed by Monte Carlo simulations. Monte Carlo simulations have three serious drawbacks for studying very unequal stiffnesses: (1) the simulated steps have only finite length, which may be close to or smaller than the correlation length; (2) the time required to equilibrate may be prohibitively long; and (3) statistical uncertainties are unavoidable. Additionally, the simulations in Ref. 2 were problematic, since $\beta A$ approached zero as $\beta B$ became large. This work avoids all those problems by finding TWDs from numerical transfer matrices with $\beta A$ held constant at $\beta B \to \infty$. This is a necessary step before the GWD can be analyzed as an ensemble average of Gruber-Mullins TWDs.

9:00AM C6.00006 Simulation of Ferromagnetic Properties for the Two-Dimensional Ising Model, CHRISTOPHER LEMON, RONALD JOHNS, Ohio Northern University — A Matlab program was written that uses Monte Carlo methods and the heat bath algorithm to simulate the two-dimensional Ising model. Several program variations were written to see if the simulation would accurately predict the existence of the Curie temperature and ferromagnetic domains. For a variety of square lattices, the net magnetization was calculated as the applied magnetic field was varied. It was found that the simulated Curie temperature is in good agreement with that predicted from the theory of the Ising model. Additionally, simulations show that lattice sites of the same spin tend to cluster together; the size of these domains is dependent on the external magnetic field. Based on these results, this program successfully simulates two hallmarks of the Ising model of ferromagnetism: Curie temperature and ferromagnetic domains.

Saturday, October 11, 2008 8:00AM - 9:12AM — Session C7 Biological Physics Oelman Hall 30

8:00AM C7.00001 Diffusion dependence of proton NMR relaxation rates in the presence of ferritin, MICHAEL BOSS, P. CHRIS HAMMEL, The Ohio State University, Dept. of Physics — Ferritin is the predominant iron-storage protein in living organisms. In aqueous solutions of ferritin, protons experience a higher transverse relaxation rate, $R_2$. This is thought to occur due to a diffusive mechanism, where protons move close enough to the ferritin to pass through a region of elevated magnetic field, and a chemical exchange mechanism, where protons bind to the protein for a period of time, experiencing an even higher magnetic field. These two mechanisms exhibit different dependencies on the self-diffusion coefficient of the protons. By adding glycerol to aqueous solutions, we have been able to control the self-diffusion of protons; this has been confirmed by means of diffusion measurements employing pulsed field gradient techniques. We have measured the relaxation rate of protons in ferritin-containing binary mixtures of water and glycerol using CPMG sequences, and will compare the experimental results to theoretical predictions of diffusion dependence.

8:12AM C7.00002 Characterization and Biocompatibility of “Green” Synthesized Silver Nanoparticles, MICHAEL MOULTON, SAMANTHA KUNZELMAN, LAURA BRAYDICHT-STOLLE, AFRL/711 HPW, M. NADAGOUDA, R. VARMA, EPA Sustainable Technology Division, SABER HUSSAIN, AFRL/711 HPW, APPLIED BIOTECHNOLOGY BRANCH, AFRL COLLABORATION, SUSTAINABLE TECHNOLOGY DIV., EPA COLLABORATION — With ever increasing emphasis on nanotechnology, silver nanoparticle are being considered for many applications in biological systems. However, the synthetic methods involve the use of potentially hazardous chemicals, extreme heat, and produce environmentally dangerous byproducts. As a culture intent on reducing our carbon footprint on the earth, societies’ focus has turned to “green” production capabilities. Therefore, if nanotechnology is to continue to grow at its current rate it is essential that novel “green” synthesis of nanoparticles becomes a reality. Furthermore, with the current and near-future applications of silver nanoparticles in biological systems it is imperative to fully analyze the potential toxic effects of these nanoparticles. In this study we have shown that by reducing silver nitrate in solutions of tea extract or epinephrine of varying concentrations spherical silver nanoparticle are formed. Furthermore, evaluation of mitochondrial function (MTS) and membrane integrity (LDH) in alveolar rat macrophages and human keratinocytes showed that these “green” synthesized silver nanoparticles were nontoxic.

8:24AM C7.00003 Mapping the energy landscape of tubulin under tension with molecular simulations, HARSHAD JOSHI, RUXANDRA DIMA, University of Cincinnati — Microtubules (MTs) play major roles in the transport of organelles in the cell and in cell division. MTs are subject to permanent tension [1] and additional forces act on MTs when external mechanical perturbations are applied to cells. To elucidate the microscopic origins of the mechanical response in MTs, we have performed simulations of a self-organized polymer (SOP) model of tubulin, the building blocks of MTs. The SOP representation is an off-lattice minimalistic description of a protein chain which allows us to perform force-induced unfolding simulations of large molecules at the loading rates and time scales of single-molecule experiments [2]. We show that the forced unfolding of tubulin involves a bifurcation in the unfolding pathways and map precise features of the complex energy landscape of tubulin by surveying the structures of the various metastable intermediates [3].

References:

8:36AM C7.00004 Computational modeling of protein folding assistance by the eukaryotic chaperonin CCT*, MANORI JAYASINGHE, GEORGE STAN, University of Cincinnati — Chaperonins are biological nanomachines that promote protein folding using energy derived from ATP hydrolysis. They are found in all the three domains of life and are grouped into two distinct classes based on their lineage. Group I chaperonins represented by GroEL of E. coli bind substrate proteins through hydrophobic interactions. By contrast, group II chaperonins are suggested to use both hydrophobic and hydrophilic interactions to recruit substrate proteins. We focus on the substrate binding mechanisms of eukaryotic (Group II) chaperonin CCT. To this end, we study the interaction of CCT with Tubulin, one of the major substrates. Using molecular docking and molecular dynamics simulations, we probe binding of the $\beta$ tubulin peptide (205-274) to the CCTγ apical domain. We identify two binding mechanisms, one involving mostly hydrophobic interactions with a helical region, which is structurally equivalent to the binding site of the bacterial chaperonin and a second one involving hydrophilic interactions with a helical protrusion region. Our results suggest that the substrate binding in CCT is highly specific, involving both electrostatic and hydrophobic interactions. These mechanisms likely to be optimized for specific substrate protein-CCT subunit pairs.

* American heart association
8:48AM C7.00005 Studies of solid DNA-CTMA films using Raman microprobe spectroscopy, FAIZAN AHMAD, PERRY YANEY, University of Dayton — Extensive research has been conducted on the development of deoxyribonucleic acid (DNA)-based electrical and electro-optical devices using purified DNA originally derived from salmon waste. However, the molecular weight of the virgin, as received DNA is greater than 8000 kDa, whereas the electrical and electro-optical properties are optimum at lower molecular weights. High power sonication is used to reduce the molecular weight of the obtained DNA to levels as low as 200 kDa, in which higher power and longer exposure produces lower mean molecular weight. The DNA is then complexed with cetyltrimethyl-ammonium chloride (CTMA) to make it water insoluble. To support the various measurements that have been made to confirm that the sonicated material is still double strand DNA and to look for other effects of sonication, Raman studies were carried out to compare the spectra over a wide range of molecular weights and to develop baseline data that can be used in correlation studies when various dopants are added to change the electrical, mechanical or optical properties. Raman microprobe spectra from solid, dry thin films of DNA with molecular weights ranging from 200 kDa to >8 MDa complexed with cetyltrimethyl-ammonium chloride (CTMA) are presented and correlated with the as-received spectrum, the CTMA spectrum and with published DNA spectra in aqueous solutions.

9:00AM C7.00006 The Bioaccumulation and Toxicity of Platinum Group Metals in Developing Chick Embryos, IOANA PAVEL, JENNIFER MONAHAN, MARJORIE MARKOPOULOS, Department of Chemistry, Wright State University, Dayton, OH 45435, USA, ZOFIA GAGNON, BRITNEY NEJAME, JACOB CAWLEY, DAVID REENS, Department of Environmental Science and Policy, School of Science, Marist College, Poughkeepsie, NY 12601, USA — Recent studies showed that platinum group metals (PGMs) such as Pt, Pd, and Rh from automobile catalytic converters, can accumulate in the soft tissues of a variety of living organisms. However, the effects of PGMs on bone and organs development of animals are not clearly understood. To examine these aspects, developing chick embryos were injected with 0.1, 1.0, 5, or 10 ppm solutions of Pt, Rh, Pd, or with a PGMs mixture. 1) Pathological Changes: were observed for all PGM treatments above 1 ppm. Bone Cells Assesment: Chondrocyte cells in tibiotarsus showed decreased diameter and length. 2) PGMs Accumulation in Tissues: was quantified by GFAAS spectrometry on finely ground tissue powder. 3) Bone Demineralization: was detected by micro-Raman spectroscopy imaging on paraffin embedded bone sections. 4) DNA Damage in Cells: was determined by using a Comet assay and fluorescence spectroscopy. Oxidative Damage in Tissues: was analyzed using a glutathione peroxidase assay. The overall results indicated that PGMs presence in our environment raises concerns about their long-term health effects on all organisms.

Saturday, October 11, 2008 8:00AM - 9:36AM — Session C8 Applied Physics and Optics Fawcett Hall 210

8:00AM C8.00001 The Bi-Directional Reflectance Distribution Function (BRDF) – Measurement and Analysis Techniques, BRADLEY BALLING, MICHAEL MARCINIAK, Air Force Institute of Technology — The Bi-Directional Reflectance Distribution Function (BRDF) either defines or represents how light reflects off a surface; it is a subset of the larger family of Bi-Directional Scatter Distribution Functions which include transmission distribution, as well. This work seeks to define and explore the BRDF through the use of both analytic and measurement techniques. Both representative and more physically based BRDF models are fit to data collected from a variety of samples using a Schmitt Industries’ Complete Angle Scatter Instrument. In particular, a measurement methodology and statistical analysis of a calibrated diffuse reflectance standard supplied by the National Institute of Standards and Technology (NIST) will be presented to demonstrate the repeatability of the measurement technique and just how much directional dependence a real-world “perfectly diffuse” reflector actually has. Analysis shows that the more physically based BRDFs do represent measured data more accurately, and hold the potential to be predictive, rather than merely a representation of previously measured surfaces.

8:12AM C8.00002 Rugged TDLAS system for High Energy Laser atmospheric propagation characterization, GLEN PERRAM, AFIT Professor of Physics, CHRISTOPHER RICE, AFIT PhD Student — An active remote sensing instrument for the characterization of atmospheric absorption, scattering, and scintillation at several key high energy laser wavelengths is in development. The instrument is based on narrow band tunable diode lasers fiber coupled to a 12” Ritchey-Chretien transmit telescope and a second receive telescope with visible or near infrared imager. For example, tunable diode lasers have been used to obtain absorption spectra in the laboratory for the Cs D2 lines near 852 nm and the oxygen X-b lines near 760 nm, key to the Diode Pumped Alkali Laser (DPAL) concept. Absorberies of less than 0.5% are observable. Applications will be assessed including effects to HEL atmospheric propagation from molecular and aerosol absorption and scattering, Cn2 estimation from atmospheric turbulence, hazardous chemical emission detection, and laser communication interception from side scattering. The system will soon be deployed to a military laser test range to characterize path lengths of greater than 1 km.

8:24AM C8.00003 Wave Optics and Prediction of Retro-reflections from Optical Systems, JOHN TATAR, WALTER COLE1, MICHAEL MARCINIAK, Air Force Institute of Technology — Optical devices interrogated with a laser in the appropriate band can exhibit strong retro-reflections of the incident beam, a characteristic that could be exploited for optical target detection and identification. The distribution of reflected power is strongly dependent on the geometry of the interrogation scenario, atmospheric conditions, and the cross section and reflectivity of the target optical device. Wave optics simulations and field tests are used to characterize the spatial distribution of reflected power from a corner cube and a lens-reflector target at varying focus.1 Currently at the US Military Academy

8:36AM C8.00004 A Transformer with Unequal Mutual Inductances, XIAODONG LIU, Department of Radiology, Washington University in St. Louis, MO 63110, USA, YU LIANG, Department of Computer Science, Michigan State University, MI 48823, USA, QICHANG LIANG, China Institute of Atomic Energy, Beijing 102413, China — We designed a new kind of transformer which is composed of a circular parallel plate capacitor and a toroidal solenoid. The toroidal solenoid is placed in the middle of the parallel plate capacitor. The circular parallel plate capacitor is used as the primary coil and the toroidal solenoid is used as the secondary coil. The toroidal solenoid could enclose air or magnetic material inside the solenoid. Numerical calculations and analyses show that this transformer has unique characteristics of unequal mutual inductances due to the displacement current. The displacement current between the plates of the capacitor contributes to the mutual inductance from the capacitor to the solenoid, while the gap between the plates reduces the mutual inductance from the solenoid to the capacitor. The mutual inductance from the solenoid to the capacitor is always less than that from the capacitor to the solenoid. This is the first transformer in the world which has unequal mutual inductances. It is anticipated that this specific device has potential applications in power transmission at radio frequency.
8:48AM C8.00005 Multipactor Discharge Mitigation in High Power Microwave, HPM, Systems, NEIL ROGERS, WILLIAM BAILEY, Air Force Institute of Technology — A multipactor discharge is an electron avalanche supported by secondary electron emission that can couple the HPM field energy to a waveguide dielectric window. The energy deposition can lead to the destruction of the dielectric material and catastrophic window failure. Mitigation approaches for this single surface multipactor at dielectric windows are investigated using Particle-In-Cell simulations. Initially baseline susceptibility diagrams are constructed analytically and compared with self-consistent, dynamic system trajectories. Geometric mitigation is then considered by varying the window design with respect to the HPM electric field. Small angular deviations, less than 20 degrees, from the nominal case of the electric field parallel to the surface show dramatic changes in the susceptibility diagram. A materials approach to mitigation is then considered. Titanium Nitride, TiN, coatings applied to the dielectric surface can substantially reduce the secondary emission yield. Representative TiN modifications of the virgin secondary emission yield are simulated and the resulting susceptibility diagrams are discussed.

9:00AM C8.00006 Bi-directional Scatter Distribution Function (BSDF) Measurements of Large Area Photonic Crystals, ROBERT LAMOTT, MICHAEL MARCINIAK, Air Force Institute of Technology, BRIAN CUNNINGHAM, University of Illinois at Urbana-Champaign — Optical metamaterials, or photonic crystals (PCs), are lattice structures made of two or more materials with different refractive indices and the structure repeating at a sub-wavelength period. This results in a photonic bandgap within the material, completely rejecting certain wavelengths, similar to an electronic bandgap within a semiconductor. Recent developments have allowed the production of PCs with large areas, suitable for an ex-situ experimental setup. In our work we utilized a two-dimensional PC consisting of a high refractive index dielectric and a low refractive index cladding material, coupled to an automated stage. In-situ micro-Raman spectroscopy and imaging is performed on the radial breathing mode and D/G bands of the growing SWNTs. The SWNTs are synthesized via thermal chemical vapor deposition on silicon substrates inside an environmental cell coupled to an automated stage. The excitation laser also serves as a localized heat source for SWNT growth. The SWNTs are grown on thermally isolated islands within the substrate and data can be collected by varying growth conditions in real time across each region. Computer control over substrate temperature, feed gas composition, chamber pressure and substrate position enable rapid exploration of the SWNT growth parameter space and the establishment of a robust database.

9:12AM C8.00007 A SWNT Synthesis Apparatus for Multivariate Analysis of Nucleation and Growth Factors, R. ACOSTA, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB and Wright State University, Department of Physics, D.C. LIPTAK, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, P. CACERES-VALENCE, University of Puerto Rico, Department of Mechanical Engineer, J. DEIBEL, Wright State University, Department of Physics, B. MARUYAMA, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB — A Multivariate analysis of various factors that influence the nucleation and growth of single-walled nanotubes (SWNTs) is demonstrated. The SWNTs are synthesized via thermal chemical vapor deposition on silicon substrates inside an environmental cell coupled to an automated stage. In-situ micro-Raman spectroscopy and imaging is performed on the radial breathing mode and D/G bands of the growing SWNTs. The excitation laser also serves as a localized heat source for SWNT growth. The SWNTs are grown on thermally isolated islands within the substrate and data can be collected by varying growth conditions in real time across each region. Computer control over substrate temperature, feed gas composition, chamber pressure and substrate position enable rapid exploration of the SWNT growth parameter space and the establishment of a robust database.

9:24AM C8.00008 Agent-Based Models for Physics and Chemistry, PAUL SEYBOLD, APS — A brief overview of the use of agent-based models for the simulation of the behaviors of complex systems will be given. It will be emphasized that these agent-based models are rules-of-thumb, rather than equations governing a quid for quasi-natural systems. Theoretical analysis and computer simulations can emerge from the simulations. Illustrations using stochastic cellular automata models of a chemicals reaction and the vapor-liquid phase transition will be presented.

Saturday, October 11, 2008 10:00AM - 12:00PM — Session D1 Plenary Session II — Fawcett Hall 101

10:00AM D1.00001 Proteins and other Foldameric Materials, KEN A. DILL, Department of Pharmaceutical Chemistry, University of California San Francisco — We have been interested in the principles that drive proteins to fold up into their uniquely biologically functional native structures. We have explored folding codes — how different types of monomer units could encode an ability to fold into a specific structure; folding kinetics — how quickly such chains can fold; and computer predictions of foldameric structures from their monomer sequences. As tests, we have explored a type of polymers, called peptides, which bear some resemblance to peptides, but have nonbiological backbones. We find that we can design such molecules to fold into helices and helical bundles, and are exploring their structures and properties. The long-term goal is new materials that could perform bio-like functions.

11:00AM D1.00002 Nanotechnology in the Environment: Lessons From and For Solid State Physics, VICKI COLVIN, Department of Chemistry, Rice University, Houston, TX 77251 — Nanotechnology-enabled systems offer great promise for solving difficult environmental and biological problems. Their small size, high surface areas, and unique properties all provide opportunity for use-driven science and engineering research. At Rice University, in a NSF research center termed CBEN, we have since 2001 been studying applications in biological and environmental engineering and the science of the “wet/dry” interface between living systems and inorganic materials. Ultimately with the appropriate tools we aim to predict the behavior – the transport, biokinetics and effects — of engineered nanoparticles in natural systems. I will give two examples of applications driven research which have exploited fundamental understanding of solid state physics in both magnetic and optical systems. Quantum dot/metal complexes, for example, can be generated to act as probes in biological systems. When linked with specific peptide sequences, these systems can detect the presence of metalloproteases or other agents. These elusive biomolecules are thought to be excellent indicators for the biological state of solid tumors, and their application could yield a combination of both structural and functional imaging. In a second example the nanoscale behavior of magnets are the basis for developing point-of-use water purification for arsenic-rich sources. High surface area and monodisperse Fe3O4 nanocrystals will move in very low magnetic field gradients (< 100 T/m) in a size-dependent fashion. The striking size dependence of the magnetic separation process permits the first multiplexed separation of nanocrystals by magnetic field strength. This phenomenon makes it possible to demonstrate in one proof-of-principle systems that high specific surface area Fe3O4 nanocrystals can be used in a magnetic separation process to remove arsenic. From these examples which are clearly cases where solid state physics taught users of nanotechnology how best to apply novel materials, I will move to lessons for solid state physics from this area of nanotechnology. Much of this discussion will center on the need for a proactive dialog about measuring the risk of technology that’s on the frontier; such debates are now a visible hallmark of nanotechnology programs worldwide. While it may seem that concerns about the health of environmental impact of nanomaterials are far from the expertise or interest of physicists, the critical role of the interface in these studies elevates the importance of surface science in particular in this emerging area. The need for more quantitative and basic studies of these interfaces in water is acute, and defines a well suited for the physics community.