

Past Physics Colloquia

Fall 2012

March 12th

Nikolay Dokholyan

Department of Biochemistry and Biophysics, University of North Carolina, Chapel Hill

Controlling Allosteric Network in Proteins

Abstract:

We present a novel methodology for delineating allosteric pathways in proteins. We use this methodology to uncover the structural mechanisms responsible for coupling of distal sites on proteins and utilize it for allosteric modulation of proteins. We will present examples where inference of allosteric networks and its rewiring allows us to "rescue" cystic fibrosis transmembrane conductance regulator (CFTR), a protein associated with fatal genetic disease cystic fibrosis. We also use our methodology to control protein function allosterically. We design a novel protein domain that can be inserted into identified allosteric site of target protein. Using a drug that binds to our domain, we alter the function of the target protein. We successfully tested this methodology *in vitro*, in living cells and in zebrafish. We further demonstrate transferability of our allosteric modulation methodology to other systems and extend it to become light-activatable.

March 5th

Michael Shlesinger

Office of Naval Research

The History of Probability Theory: Predicting the Unpredictable

Abstract:

This lecture traces the history of probability theory from the throwing of bones, sticks, and dice to modern times. Early 18th century books, Jacob Bernoulli's "The Art of Conjecture" and Abraham DeMoivre's "The Doctrine of Chances" were rich with new mathematics, insight and gambling odds. Progress was often made by confronting paradoxes. The first of these confused probabilities with expectations and was explained in the Pascal-Fermat letters of 1654. The St. Petersburg Paradox involved a distribution with an infinite first moment, and Levy discovered a whole class of probabilities with infinite moments that have found a surprising utility in physics. The Bertrand paradox involved measure theory for continuous probabilities, Poisson discovered that adding random variables need not always produce the Gaussian, and Daniel Bernoulli and D'Alembert argued over the probabilities for the safety of smallpox vaccinations. Using these and other anecdotes, this lecture discusses vignettes that have brought us to our modern understanding of probability theory.

February 26th

Nickolay Korabel

Department of Physics, University of California, Merced
Department of Bioengineering, Stanford University

Intracellular Transport: the Role of Cytoskeleton Topology

Abstract:

The eukaryotic cytoskeleton is composed of polarized filaments forming a complex, intertwined network. Various motor proteins such as kinesins or myosins convert ATP into mechanical work and are able to walk processively or even diffuse along the cytoskeleton. Large organelles such as vesicles or mitochondria can randomly bind and unbind to one or several motors and their transport in the cell can be described as alternating phases of diffusion in the cytoplasm and phases of directed or diffusive transport along the cytoskeletal network.

Intracellular transport has been the focus of extensive studies both experimentally and theoretically. However, the impact of the cytoskeleton network structure on transport properties, which is expected to be significant, is not fully understood. We develop a computational model of intracellular transport, and explore the impact of the cytoskeletal structure on transport properties. We show that transport can be enhanced even by diffusional motion along the cytoskeleton after memory effects due to cytoskeletal structure are taken into account. We also explore the influence of the network structure on the first passage time distributions for a cargo to reach the cell membrane after being exported from the nucleus and for transport from the membrane to the nucleus.

February 19th

Boris Shapiro

Technion (Israel Institute of Technology)

The discussion will focus on three topics:

1. A disorder induced superfluid-insulator transition.
2. Dynamics of cold atoms in the presence of a random potential, and the related issue of the Anderson localization.
3. Free expansion of a condensate with an initial density modulation and possible developments of matter wave caustics.

February 12th

Levent Kurt

Division of Mathematics and Natural Sciences

A Quantitative Approach to the Switching Strategies and Emotions of Disputants in a Conflict

Abstract:

The time series like data resulted from social experiments may be studied further quantitatively using mathematical and statistical analysis as well as physical models. We study the dynamics of conflict between disputants who were engaged in a discussion on a socio-political topic such as death penalty, affirmative action, abortion or euthanasia. The two kinds of data, namely, emotion and behavior data, are analyzed using some well-known techniques such as Hurst rescaled range analysis. The probability density function (PDF) of the switching behaviors of the participants turn out to be stretched exponential distribution. Such form of the PDF has been used to describe many physical phenomena such as the discharge of a capacitor and remanent magnetization in spin glasses. The stretched exponential PDF is an indication of memory in the way people behave and, therefore, behavioral dynamics are non-markovian process. To point out this result more rigorously, we also derive an analytical solution for the effective rate constant based on the stretched exponential form of PDF. The effective rate constant may be used as the measure of switching behavioral states as it is also used as the probability that a light bulb fails to produce light given that it has already produced light for t amount of time renewal theory. As oppose to behaviors, emotions seem to flow in a random way. Not only Hurst rescaled range analysis resulted in Hurst exponent being 0.5, which is an indication of random process, within the range of zero to one, but also Power spectrum analysis confirms that the dynamics is just random process or classical Brownian motion.

February 5th

Valerie Halyo

Department of Physics, Princeton University

There and Back: the Journey to find the Higgs at the LHC

Abstract:

Nearly 50 years have passed since the work describing the Higgs particle as the one responsible to give mass to the gauge fields was suggested. These years were spent with tireless efforts of thousands of experimentalists around the world searching for the scalar particle called the Higgs boson. Not only would the discovery of the Higgs particle yield the missing link to the present Standard Model theory of elementary particles, but a detailed analysis of the decays would possibly yield information about the spectrum beyond the Standard Model.

The goal of the first run at the Large Hadron Collider (LHC) was to find the Higgs with the first 15 fb^{-1} of data. However both collaborations CMS/ATLAS already managed to observe a Higgs-like particle with the first 5 fb^{-1} of the data recorded. The results were announced at an historic event on July 4, 2012 in Melbourne, Australia. However the question is---Is it the Standard Model Higgs or is it a Higgs-like particle?

January 29th

Valery Nesvizhevshy

Institute Laue Langevin, Grenoble, France

Quantum States of Matter and Anti-matter in Gravitational and Centrifugal Potentials

Abstract:

Two phenomena have been observed recently in experiments with slow neutrons: quantum states of ultracold neutrons (UCN) in the Earth's gravitational field [1] and quantum states of cold neutrons (CN) in the centrifugal potential in the vicinity of a curved mirror [2]. The first experiment presented the first observation of quantum states of matter in a gravitational field; the second one is also known as the neutron whispering gallery effect. They are related by common experimental methods used, by common mathematical description, but also by their applications in elementary particle physics, in quantum optics, in surface science [3]. It is curious that these experiments present the first direct demonstration of the weak equivalence principle for an object in a quantum state. Much more precise measurements of/with these phenomena are going to be performed in a recently constructed second-generation GRANIT spectrometer [4]. Analogous experiments could be probably performed in future with anti-matter atoms [5-6], with interesting applications in various domains of science.

December 4th

Jean Bellissard

School of Mathematics and School of Physics, Georgia Institute of technology

Atomic Motion in Aperiodic Solids: the Case of Liquids and Glasses

Abstract:

After reviewing some examples of aperiodic solids, and some of their properties, the concept of Hull will be introduced. Based upon recent results on the properties of liquids and glasses, the concept of Delone graph and of edge stress will be introduced in order to define a thermal equilibrium state. The equilibrium dissipative dynamics will also be described in terms as precise as possible at the time of the talk. A discussion of the expectations from such an approach will conclude the talk.

November 27th

Alexander Lisyansky

Queens College, CUNY

Quantum Plasmonics of Metamaterials: Perspectives of Loss Compensation with Spasers

Abstract:

There are a lot of expectations that spasers can be used for loss compensation in metamaterial. This immediately calls for a study of spasers' behavior in the external field, which I will discuss in my talk. A spaser is an autonomic non-linear oscillating system, and therefore, its response to a periodic perturbation is not easily predictable. E.g., even extremely low field can drive a spaser into stochastic oscillations. Nonetheless, I will demonstrate that under certain conditions spaser can provide exact loss compensation. I will also discuss cooperative phenomena showing that in a chain of interacting spasers either all spasers oscillate in phase or a nonlinear autowave travels in the system. In the latter scenario, the traveling wave is harmonic, unlike excitations in other nonlinear systems. Due to the nonlinear nature of the system, any initial distribution of spaser states evolves into one of these steady states.

November 13th

Mikhail Anisimov

Institute for Physical Science and Technology

Department of Chemical and Biomolecular Engineering, University of Maryland, College Park

Entropy-Driven Liquid-Liquid Transitions in Pure Substances

Twenty years ago Poole *et al.* [1] suggested that the anomalous properties of supercooled water may be caused by a critical point that terminates a line of metastable liquid–liquid separation of lower-density and higher-density water. The hypothesized existence of two liquid states in pure water can be globally viewed in the context of liquid polyamorphism, a phenomenon that has been experimentally observed or theoretically suggested in silicon, liquid phosphorus, triphenyl phosphate, and in some other molecular-network-forming substances [2]. We have developed a phenomenological model in which liquid water at low temperatures is viewed as an ‘athermal solution’ of two hydrogen-bond network structures with different entropies and densities [3]. Alternatively to lattice-gas models, in which fluid phase separation is driven by energy, the phase transition in the athermal two-state water is driven by entropy upon increasing the pressure, while the critical temperature is defined by the ‘reaction’ equilibrium constant. The order parameter is associated with the entropy, while the ordering field is a combination of temperature and pressure. The model predicts the location of density maxima at the locus of a near-constant fraction of the lower-density structure.

Another example of entropy-driven liquid polyamorphism is the transition between the structurally ordered ‘Blue Phase III’ and disordered liquid in some chiral materials [4]. Thermodynamics of this transition is remarkably similar to that of the hypothesized liquid-liquid transition in supercooled water. However, unlike the metastable transition in supercooled water, the transition between the Blue Phase III and ordinary liquid state is located in the stable region and is experimentally accessible.

[1] Poole, P. H., Sciortino, F., Essmann, U. & Stanley, H. E. “Phase behaviour of metastable water”, *Nature (London)* **360**, 324 (1992).

[2] McMillan, P. F. “Polyamorphic transformations in liquids and glasses”, *J. Mater. Chem.* **14**, 1506 (2004).

[3] Holten, V. & Anisimov, M. A. “Entropy-driven liquid–liquid separation in supercooled water”, *Sci. Rep.* **2**, 713 (2012). <http://www.nature.com/scientificreports>

[4] Anisimov, M. A., Agayan, V. A. & Collings, P. J. “Nature of the Blue-Phase-III isotropic critical point: An analogy with the liquid-gas transition”, *Phys. Rev. E* **57**, 582–595 (1998).

October 23rd

Steven Eppell

Case Western Reserve University

Using Nanotechnology to Determine Strain Fields Seen by Single Cells

Abstract:

Predicting mechanical behavior of biological materials like bone and tendon is important when developing clinical methods used to determine mechanisms resulting in tendonitis and risk of fracture in disease states like osteoporosis. This prediction requires application of multiscale models which use as inputs constitutive parameters of the individual structures within the hierarchy of the material. These parameters, especially strength and viscosity, are not well known at the 100 nm length scale for any collagenous material. The structure at this length scale is called a fibril. We used a method based on Microelectromechanical Systems (MEMS) technology allowing in-fluid uniaxial tensile tests on such fibrils. Our data matches a multiscale molecular dynamics simulation. The data shows that individual fibrils strain to ~80% before rupturing displaying a strength of ~230 MPa. These values are ~5X greater than whole tendon indicating that tendon failure mechanisms likely involve the non-collagenous phases of the tissue in important ways.

October 16th

Igor Lubomirsky

Weismann Institute of Science

Elastic and Electric Anomalies in Solids

Abstract:

In many solids and particularly in ionic conductors, the concentration of point defects can reach 10^{21} - 10^{22} cm⁻³, which comprises a few percent of the total number of atomic sites. This concentration is sufficiently high that interaction of point defects may strongly affect the elastic and electromechanical properties of the solids. We investigated the elastic behavior of thin films of oxygen-deficient ceria and Gd-doped ceria as examples of solids with a very large concentration of interacting point defects. We showed that in these films externally applied mechanical stress may be partially relieved by a shift in the association/dissociation equilibrium of the point defects. Association/dissociation of the point defects in response to external stress proceeds until the decrease in elastic energy is balanced by the increased chemical energy of the defect distribution. The resulting change in linear dimensions may be called "chemical strain", in analogy to the previously studied "chemical stress". We have recently shown that Gd-doped ceria can generate stress comparable to or surpassing the best commercial piezoelectrics and electrostrictors currently in use. Using local structure measurements by EXAFS and XANES we found that both CeO_{2-x} and Gd-doped ceria preserve their lattice (fluorite) symmetry only on average. Locally, a high concentration of oxygen vacancies causes the lattice to undergo local distortion due to the weakness and lability of the cerium-vacancy interaction. Moreover, the lability of this interaction allows for facile rearrangement of the distorted units, which can be driven by either mechanical stress or by an external electric field. This microscopic mechanism is expected to be common for a variety of solids with a large concentration of point defects and may be useful in the design of new engineering materials.

September 11th

Ying Wang

Massachusetts Institute of Technology

Phase Transitions in Antibody Solutions: from Pharmaceuticals to Human Disease

Abstract:

Antibodies (immunoglobulins) are very important proteins. Natural antibodies play an essential role in the immune system of the human body and pharmaceutical antibodies are used as drugs. Antibodies are also indispensable tools in biomedical research and diagnostics. Recently, the biopharmaceutical industry became interested in antibody formulations with very high concentrations (up to 100mg/mL). Consequently, a number of observations of phase transitions (i.e., crystallization and liquid-liquid phase separation) of pharmaceutical antibodies have been reported. These phase transitions are undesirable from the perspective of colloid stability of drug solutions in processing and storage, but can potentially be used for improving pharmacokinetics of drugs. Furthermore, phase transitions, especially crystallization, of antibodies are useful in applications such as protein purification and X-ray crystallography. Phase transitions of immunoglobulins can also take place in the human body, particularly in multiple myeloma patients who overproduce monoclonal antibodies. These antibodies may, in some cases, crystallize at body temperature and cause severe complications (cryoglobulinemia).

In this talk, I will present the results of our current studies on phase transitions of both pharmaceutical antibodies and cryoglobulinemia-associated antibodies. These studies have shown that different antibodies have different propensity to undergo phase transitions, but their phase behavior has universal features which are remarkably different from those of spherical proteins. I will discuss how studies of phase behavior can be useful in assessing colloid stability of pharmaceutical antibodies and in early diagnostics of cryoglobulinemia, as well as general implications of the fact that some antibodies can precipitate at physiological conditions.

August 28th

Alexander Kolobov

Phase-change Memory Alloys: Current Status and Future Challenges

Abstract:

GeTe-based alloys, primarily along the quasibinary GeTe-Sb₂Te₃ tie-line (GST), exhibit unusually large property contrast between the crystalline and amorphous phases. combined with high switching rates between the two and high stability of both phases. This unique combination of properties makes them ideal materials for memory applications, such as re-writable DVDs and nonvolatile electronic memories, so-called phase-change random access memory (PC-RAM).

In this talk, first, the author's experimental and computational studies of the structure of the crystalline and amorphous phases are reviewed, followed by a discussion of the phase-change mechanism, including the role of electronic excitation.

The talk is concluded by describing future trends in phase-change memories such as interfacial phase-change memory (iPCM) with substantially reduced energy consumption and the initial studies on applying topological insulator properties of iPCM to developing novel memory devices combining the merits of phase-change and magnetic memories.

Spring 2012

May 8th

Wei Ku

CMPMSD, Brookhaven National Laboratory Upton, NY 11973, USA
Physics Department, Stony Brook University, Stony Brook, NY 11790, USA

Iron-based high-temperature superconductors, a new "favorite" family in condensed matter physics

Abstract:

Recent discovery of iron-based high temperature superconductors has generated intense research activities in the fields of condensed matter physics, materials sciences and physical chemistry. While only very limited solid understandings have been obtained and more puzzles are being unveiled, it has become clear that this new class of materials is a perfect host for the complex and rich condensed matter physics involving multiple physical effects with similar energy scales.

This talk will present a general introduction of some of the modern topics of condensed matter physics, and why high-temperature superconductivity is particularly of interest. The talk will then cover the simple idea of density functional theory, one of the most powerful theoretical tools for real materials. Finally, a few current issues concerning the Fe-based superconductors will be addressed, illustrating the rich physics in this new class of superconducting materials.

May 1st

Shane Huston

Putting Models of Morphogenesis to the Test Using Laser-Microsurgery

Abstract:

The biological tissues of a developing organism are built and reshaped by the mechanical behavior of individual cells – a process known as morphogenesis. Physicists have contributed to our understanding of morphogenesis largely through the construction of computational models. These models typically posit a temporal sequence of cellular mechanics – possibly with some feedback mechanisms – that reproduce the observed sequence of cell and tissue deformations. Unfortunately, even for a well-defined set of deformations, a single model is not a unique solution. To test whether

specific computational models are biologically relevant, we have developed methods to probe cellular mechanics *in vivo* using laser-microsurgery – both qualitatively, to assess whether removal of specific cells alters the dynamics of tissue reshaping, and quantitatively, to measure sub-cellular mechanical properties and stresses. I will detail two types of quantitative microsurgical measurements: one based on drilling holes in sheets of epithelial cells; and a second that mechanically isolates a single cell using holographically shaped laser pulses. The subsequent retraction (or expansion) of the isolated cell allows one to separate and quantify the effects of intra- and intercellular stresses. I will discuss application of these techniques to the time-dependent biomechanics of epithelial tissues in developing fruit fly embryos.

April 17th

Olga Safonova

Paul Scherrer Institute, Villigen 5232, Switzerland

X-rays as a Powerful Tool for the Structural Studies of Working Catalysts and Applied Materials on the Atomic Scale

Abstract:

Synchrotron radiation offers a number of X-ray based techniques for the structural studies of applied materials. Compared to laboratory X-ray sources the intensity of X-ray beams at modern synchrotrons is by orders of magnitude higher. It allows increasing energy-, spatial- and time-resolution of well-known diffraction and scattering techniques and developing of new methods with enhanced chemical sensitivity. The intense X-ray beams are also particularly suitable for *in situ* studies of the dynamic structure of working catalysts, fuel cells, gas sensors etc. Several examples showing the advantages of modern X-ray science for the studies of structural transformations in metal nanoparticles, oxides, and amorphous metals will be discussed.

April 3rd

Diana Farkas

Professor Materials Science and Engineering, Virginia Tech, USA

Computer Simulation Studies of Deformation Mechanisms and Ductility in Nano Crystalline FCC Materials

Abstract:

Molecular dynamics computer simulation techniques were used to conduct virtual tensile tests in samples containing random tilt grain boundaries and an average grain size of 40nm. The mechanisms of plastic deformation resulting from the tensile straining were analyzed in detail. We utilized empirical interatomic potentials and analyze the critical role of the sample geometry and microstructure in determining overall mechanical response. The effect of H impurities segregated to grain boundaries is also studied. The results show that the samples containing the H impurities

show decreased overall ductility, due to increased crack nucleation at the boundaries and triple junctions.

March 27th

Walter Strauss

Math Department, Brown University, USA

Steady Rotational Water Waves

Abstract:

The mathematical study of water waves began with the derivation of the basic mathematical equations of fluids by Euler in 1752. Later, water waves played a central role in the work of Poisson, Cauchy, Stokes, Levi-Civita and many others. It remains a very active area to the present day.

I will consider a classical 2D traveling water wave with vorticity. By means of local and global bifurcation theory using topological degree, we now know that there exist many such waves (exact solutions of the Euler equations with the physical boundary conditions) of large amplitude. This work is joint with Adrian Constantin. I will also exhibit some numerical computations of such waves, obtained jointly with Joy Ko. Even after two and a half centuries many fundamental problems remain open.

March 20th

Tanya Zelevinsky

From Precision Metrology to Dark Matter Detectors with Ultra-Cold Atoms and Molecules

Abstract:

We will discuss ongoing and planned measurements with laser-cooled atoms in magneto-optical traps and in optical lattices. Progress toward preparing and manipulating ultracold molecular dimers and using them for a molecular clock, or frequency & time standard, will be presented. We will describe the applications of this research to fundamental physics questions such as dark matter detection and stability of the electron-proton mass ratio.

February 21st

Valentin Afraimovich

Professor - Researcher, IICO, Universidad Autonoma de San Luis Potosi, S.L.P., Mexico

Sequential Behavior in Dynamical Networks

Abstract:

Dynamical networks are mathematical models that describe an activity of biological, cognitive and other real systems. They consist of active elements possessing their own dynamics joined together by different types of couplings. There are a variety of forms of behavior in dynamical networks. Among them one can single out processes that are accompanied by short-time activity of individual elements or small groups of elements. Such a behavior is called sequential dynamics. It is related to the existence in the phase space of the full system of a collection of metastable sets joined by heteroclinic trajectories. The sequential dynamics can be thought of as the process of successive switching among these metastable sets. In the talk, it is supposed to discuss the simplest case, i.e. to describe main ideas and results in the situation where all metastable sets are represented by saddle equilibrium points. The talk is based on the works with the group of M.I. Rabinovich (UCSD) that started with [1,2] and still in progress [3].

Literature.

1. V.S. Afraimovich, M.I. Rabinovich, P. Varona, Heteroclinic contours in neural ensembles and the winnerless competition principle, *Int. J. Bifurcat. Chaos*, (2004), 1195-1208
2. V.S. Afraimovich, V.P. Zhigulin, M.I. Rabinovich, On the origin of reproducible sequential activity in neural circuits, *Chaos* (2004), 1123-1129
3. M.I. Rabinovich, V.S. Afraimovich, C. Bick, P. Varona, Information flow dynamics in the brain, *Phys. Life Rev.*, doi:10.16/j.plev.2012.01.002

February 14th

V. Parameswaran Nair

Particles, Plasma and Feynman's Last Problem

Abstract:

I shall review some particle physics, focusing on the standard model, then talk about some aspects of the quark-gluon plasma. One of the theoretical problems which arises in this context, among many, is the high temperature limit of the theory. This was essentially the last problem in physics which Richard Feynman worked on. I shall review what progress we have made using some of his ideas.

February 9th

Jimena Canales

A Tenth of a Second

Abstract:

In the late fifteenth century, clocks acquired minute hands. A century later, second hands appeared. But it wasn't until the 1850s that instruments could recognize a tenth of a second, and, once they did, the impact on modern science and society was profound. Revealing the history behind this infinitesimal interval, *A Tenth of a Second* sheds new light on modernity and illuminates the work of important thinkers of the last two centuries.

Fall 2011

December 13th

Ralph Nuzzo

University of Illinois Urbana-Champaign

Functional Materials and Enabling Fabrication Methods for High Performance, Low-Cost Energy Systems

Abstract:

The fabrication of high performance integrated circuits provides examples of the most sophisticated manufacturing methods, as well as the most high performance materials, used in an area of modern technology. The advanced functional systems they provide are ones that are generally characterized by a massive integration of circuit elements within compact, rigid and essentially planar form factor devices. New means of fabrication and enabling materials are beginning to provide a set of means through which it is possible to lift some of these latter constraints—doing so in ways that both retain capacities for high performance while enabling new, low cost opportunities for use in technology. Our collaborative research here at the University of Illinois is providing form factors for devices with interesting but what had been to date difficult to realize features. Examples include: light weight, large area, high performance electronics, optics, and photonics; electro optical systems with curvilinear shapes and capacities for accommodating demanding forms of mechanical flexure; and hybrid systems for lighting, energy storage, and photovoltaic energy conversion that might provide potentially transformational approaches to supplant current technologies with high performance, low cost alternatives. In this lecture I will explore examples of energy technologies enabled by new form factors for devices, highlighting three exemplary cases where opportunities for progress have benefitted from a reexamination of the modes for incorporating highly functional electronic materials into advanced, fully integrated

modules.

December 6th

Hugo Fort

Universidad de la Republica, Montevideo

Solving the Traveling Salesman Problem

Thermodynamic versus Darwinian Methods

November 29th

Seongshik Oh

Rutgers University, Piscataway

Engineering Materials One Atom Layer at a Time

November 22nd

Myriam Sarachik

City College of New York, City University of New York, USA

Molecular Magnets: A Rich Playground for Fundamental Physics

Abstract:

Molecular magnets are interesting materials that display macroscopic (more correctly, *mesoscopic*) quantum tunneling of magnetization, spin-Berry phase interference, thermally-controlled transitions from classical (thermally-activated) to purely quantum mechanical spin reversal, spin reversal by magnetic avalanches, and effects associated with the presence of random fields. With the help of animations, we will begin with a basic description of the unusual structural and magnetic properties of molecular nanomagnets using Mn₁₂-acetate as a prototypical example, and then offer a quick tour of the fascinating physical processes that have found expression in these materials.

November 5th

Shlomo Havlin

Bar Ilan University, Israel

The Theory of Complex Networks

October 4th

John H. Lowenstein
New York University

Renormalization in Chaotic and Pseudochaotic Dynamical Systems

September 27th

Daniel Visnivesky
UNICAMP, State University of Campinas, Brazil

The Dirac I met at Yeshiva University in 1965

September 20th

Guillermo Quinteiro
Departamento de Fisica, Universidad de Buenos Aires, Argentina

Interaction of Twisted Light with Semiconductors

Abstract:

The recent development of techniques to generate beams of twisted light --or light carrying orbital angular momentum-- has boosted the study on many aspects of this peculiar type of radiation. Research involving twisted light has been carried out in numerous areas, such as generation of twisted beams, interaction of OAM beams with mesoscopic particles, entanglement between spin and OAM for potential applications to quantum-information science, etc. Nevertheless, the problem of the interaction of TL with condensed matter systems is largely unexplored. In this talk I will present our theoretical investigation on the effects that twisted light has on bulk semiconductors and semiconductor nanostructures, i.e. quantum dots and rings. By studying the evolution of the electronic population and coherence, we predict that the transfer of orbital angular momentum from the light to the material produces electric currents and magnetic fields. In the case of quantum dots, we analyze the optical matrix elements and conclude that new non-vertical transitions are possible. For interband transitions in quantum rings we predict non-vertical Rabi oscillations; for intraband transitions we describe new effects when the Rasha spin-orbit coupling is considered. Finally, potential applications are discussed.

Spring 2011

April 12th

Francesca Tria
ISIF, Torino, Italy

Complexity

April 5th

Igor Sokolov
Humboldt-Universität zu Berlin

Non Equilibrium Systems

March 29th

Gabriel Cwilich
Yeshiva University, USA

Fluctuations in Intensity as a New Subwavelength Microscopy Tool

Abstract:

When a wave propagates coherently in a disordered system interesting spatial and angular correlations appear both between the fields and the intensities in the different transport regimes (ballistic, diffusive, localized) due to the interference between the different trajectories of the propagating wave in the random medium.

Effects of interference have also been studied in the Hanbury Brown-Twiss geometry in media without disorder, both in the stellar case and in quantum optics systems, to obtain information about the sources.

Here we discuss for the first time the coherent propagation in a random medium of several sources in that geometry using random matrix theory, and we find new interference effects beyond the traditional Hanbury Brown-Twiss correlations, which opens the door to the possibility of spectroscopy in subwavelength scale lengths.

March 22nd

Moniek Tromp
University of Southampton, USA

Catalysts in Action: New Developments in X-ray Spectroscopy Providing More and Faster Insight

Abstract:

Selective x-ray absorption spectroscopy (XAS) techniques, both theory and instrumentation, are currently being developed and applied to catalytic systems. The properties and catalytic performance

of homogeneous and heterogeneous catalysts are studied during their synthesis and activity, with a combination of complementary (spectroscopic) techniques. The influences of different ligands and/or supports on the structural and electronic properties of the active site are investigated. Detailed insights in reaction mechanisms, including (enantio) selectivity, are obtained.

In this lecture the different X-ray techniques and developments are described, including set-ups to allow in situ or operando experimentation, and applied to a range of important homogeneous and heterogeneous reactions.

March 1st

Amitai Bin-Nun

University of Pennsylvania, USA

Black Holes and Hidden Dimensions in String Theory

Abstract:

Gravitational Lensing is the study of light bent by a gravitational field. This effect has been known, but only studied in the weak field regime. In the last decade, there has been renewed interest in the lensing effects of compact objects such as black holes. In this presentation, I will give a conceptual overview of gravitational lensing and discuss the relevance of gravitational lensing by black holes. In particular, I will discuss the implications for observations of the center of the Milky Way galaxy, a topic of intense research interest.

September 22nd

Sijue Wu

University of Michigan

Wellposedness of the Two and Three Dimensional Full Water Wave Problem

We consider the question of global in time existence and uniqueness of solutions of the infinite depth full water wave problem. We show that the nature of the nonlinearity of the water wave equation is essentially of cubic and higher orders. For any initial data that is small in its kinetic energy and height, we show that the 2-D full water wave equation is uniquely solvable almost globally in time. And for any initial interface that is small in its steepness and velocity, we show that the 3-D full water wave equation is uniquely solvable globally in time.

October 12, 2010 Anatoly Frenkel (Yeshiva University) Electronic, structural and thermal properties of nanocatalysts non-metal, non-bulk and non-Debye

Negative thermal expansion, a peculiar effect reported in some framework solids and unexpected in close packed structures was recently (2006) observed in Pt nanoparticles. In subsequent years, more experimental information on the structure, electronic properties and dynamics of nanometer-scale clusters was obtained for different sizes, support materials, alloying elements and adsorbates. In this talk we focus on vibrational properties of supported Pt clusters that revealed markedly non-Debye behavior. We demonstrate how to explain many anomalies by the effects of the shape, size, morphology, adsorbates and the substrate. Cumulatively, these findings open a new approach to understanding the mechanism of catalytic activity of metal clusters.

October 19, 2010 Amish Khalfan, Yeshiva University Mass Relations for the Quark-Diquark Model and an Algebraic Realization

There is good phenomenological evidence to suggest that in a rotationally excited baryon (a system of three quarks), a quark - diquark structure ($q - D$) is favored over a three quark structure ($q q q$) for light quarks. At large spin, two of the quarks form a diquark ($D = qq$), a bilocal object at one end of a spherical bag with the remaining quark being at the other. The underlying quark-diquark symmetry leads to a supersymmetric $SU(6/21)$ symmetry between mesons and baryons. We will show a derivation of hadronic mass formulae based on the quark-diquark symmetry to obtain a result which is in good agreement with experiment. We will discuss the algebra of the octonions, an eight-dimensional non-associative algebra, and understand how to multiply the unit octonions via the use of the theorems of Desargues and Pappus. We can construct split-octonions, or linear combinations of the unit octonions, to provide an algebraic description of color degrees of freedom leading to the existence of exotic meson states (quark-antidiquark), for which now there is a good deal of experimental evidence.

October 26, 2010 Zafar Iqbal (New Jersey Institute of Technology) Enzymatic Biological Fuel Cells with Carbon Nanotube Electrodes

In this talk I will introduce the fundamentals and brief overview of Pt-catalyzed hydrogen fuel cells and enzymatic biological fuel cells or biofuel cells [1]. This will be followed by a discussion of work on biofuel cells from my group at the New Jersey Institute of Technology (NJIT) and in collaboration with Prof Frenkel's group at Yeshiva. Biofuel cells engineered on a molecular scale provide a continuously renewable, tailored power source for a wide range of applications, including: targeted drug delivery, physiological monitoring and control, synthetic organs, prostheses, and other advanced medical devices, which include pacemakers, insulin pumps, glucose and pressure sensors, and bionic devices for stimulating the brain and spinal cord. With growing advances in medicine, there is an increasing trend towards the use of implantable electrical devices, which require renewable power without the need for maintenance requiring surgery. Implanted biofuel cells would use natural fuel and oxidants in the body's blood stream, such as glucose and oxygen, respectively, and convert them to essentially benign byproducts with the generation of electricity. Biofuel cells can also operate as biosensors for monitoring glucose levels in the body.

November 2, 2010 Sioan Zohar, Applied Science Innovations

We present our research into the magnetization dynamics of ultra-thin polycrystalline NiFe/Cu/CoZr trilayers and superparamagnetic Iron-Oxide nanoparticle thin films. In the NiFe/Cu/CoZr trilayers, we observe evidence for pure spin current propagation similar to evidence observed in previous studies on epitaxial Fe/Au/Fe trilayers. In the Iron-Oxide nanoparticle thin films, we have observed a magnetic resonant frequency for field relation similar to those found in ferromagnetic thin films. We show that modifying the Kittel field for frequency condition to account for an unsaturated magnetic moment adequately models the magnetization dynamics. Additionally, we present our advancements in x-ray/xfi instrumentation accomplished over the course of these investigations. These advancements have decreased x-ray detected magnetic resonance acquisition times by over an order of magnitude, and provided "proof of concept" for future work aimed at probing magnetization dynamics with simultaneous nanometer and nanosecond resolution.

November 30, 2010 David Huse, Princeton University Many-Body Anderson Localization vs. Thermalization: Heat Bath Failure

An isolated strongly-interacting system of many spins, qubits, or particles with static disorder may be many-body localized at high temperatures. In that case it fails to relax to thermal equilibrium, even in the long-time limit. There is a quantum phase transition at nonzero temperature between the "ergodic" phase, where the system does thermalize and serves as its own heat bath, and the localized (or glass) phase, where the infinite system fails to be a heat bath so equilibrium quantum statistical mechanics no longer captures the long-time averages and the thermal conductivity vanishes.

Tuesday, January 26, 2009 Andrea Piovano (Università di Torino) Solid Oxide Fuel Cells: Advantages, Challenges, and Physicist's Approach to Solving Them

The requirements for new and clean power supplies, such as solid oxide fuel cells (SOFCs), have stimulated considerable research activities in the last decades on solid oxygen ion conductors operating at moderate temperatures. The need of low working temperatures is related both to the degradation problems happening at higher temperatures and to the possibility to use them in automotive applications. In this regard, non-stoichiometric perovskite-type oxides, as $\text{SrMO}_{2.5}$ ($M=\text{Co,Fe}$), are particularly interesting as they are able to undergo a reversible topotactic oxygen intercalation reaction, via electrochemical oxidation in an aqueous alkaline electrolyte, even at room temperature, following the reaction scheme: $\text{SrMO}_{2.5} + x \text{O}_2 \rightarrow \text{SrMO}_{2.5+x} + 2x \text{e}^-$ ($0 < x < 0.5$) ($M = \text{Co, Fe}$) (1). The scientific interest on this material is twofold: from one side is fundamental to characterize these structure during a real electrochemical reaction, in order to be able to extract phases that play a role in that and identify their structural and electronic properties. From the other the aim is understand the forces that drive this low temperature ionic migration inside a dense lattice. We believe that ionic conduction may be aided by specific low energy lattice vibrations. To answer to the first need we followed reaction (1) by XAFS during in situ electrochemical reaction, using an ad hoc conceived cell optimized to minimize the thickness of the solution, which is highly absorbing at the Co (Fe) K-edge. A complete evolution of the Co (Fe) local environment and of the oxidation state of the transition element as a function of the charge transfer x has been obtained from this study. Analogies and differences between the two systems are discussed.

Furthermore to understand the soft-mode driven oxygen diffusion phenomenon we analyzed the counterpart system $\text{CaFeO}_{2.5}$, which at room temperature has no conduction but starts over 800°C , in the form of single-crystal by means of Inelastic Neutron Scattering at different temperatures. This technique is the most suitable to extract low energy vibration information in the whole first Brillouin Zone. Obtained results show some vibrational softening that could be the key to understand effectively low temperature ionic conduction phenomenon.

During the presentation a survey on fuel cells, their chemistry of reaction and a detailed description of the techniques applied, inclusive of physics behind them, will be done.)

**Monday, February 1 2009 at 8 pm 218 BELFER HALL Leigh Hochberg (Brown University)
Turning Thought into Action: Brain-Computer Interfaces and Restorative Neurotechnologies
Note: Special Day, Time and Place**

For people with cervical spinal cord injury, brainstem stroke, amyotrophic lateral sclerosis (ALS, Lou Gehrig's disease) and other neurologic illnesses, currently available assistive and rehabilitation technologies are inadequate. In severe brainstem stroke and advanced ALS, both the ability to speak and the ability to move are lost, creating a "locked-in" state of being awake and alert but unable to communicate. Neural interfaces, however, are poised to revolutionize our ability to restore lost function to people with neurologic disease or injury. Over the past decade, technologies to record the individual and simultaneous activities of dozens to hundreds cortical neurons have yielded new understandings of cortical function in movement, vision, cognition, and memory. This preclinical research, generally performed with healthy, neurologically intact non-human primate subjects, has demonstrated that direct neural control of virtual and physical devices can be achieved. Recently, this exciting research has been translated into initial pilot clinical trials of the BrainGate2 Neural Interface System (IDE), seeking to determine the feasibility of persons with tetraplegia controlling a computer cursor simply by imagining movement of their own hand. A variety of methods for recording and decoding brain signals are now being tested, with the hope of not only restoring communication, but also providing a control signal for the reanimation of paralyzed limbs.

Tuesday, February 9 2009 Taylor Hughes (U. of Illinois Urbana Champaign) Time Reversal Invariant Topological Insulators and Superconductors

Nearly three decades ago the integer quantum Hall effect provided experimentalists an extraordinarily accurate way to measure the integers. With the recent experimental discoveries of the 2d and 3d time-reversal invariant Z_2 topological insulators an open question remains: how can we measure this Z_2 number? In this talk I will discuss a natural generalization of the integer quantum Hall effect and how it subsequently leads to physical, electromagnetic ways to measure the Z_2 invariant in two and three dimensions. These topological insulators have topological superconducting relatives which have interesting properties that I will discuss. In addition to this I will indicate how superconductor and ferromagnetic proximity effects can be used to mimic many of these interesting topological systems in light of the ground breaking work done by L. Fu and C.L. Kane.

Tuesday, February 16 2009 Nicolas Giovambattista (Brooklyn College) Hydration and Phase Behavior of Water in Nano-Scale Confinement

We present molecular dynamics simulations of (i) water confined by nano-scale hydrophobic, hydrophilic, and "patchy" plates; (ii) water confined by protein surfaces; and (iii) water in contact with infinite walls. At fixed temperature, water confined between hydrophobic plates can form vapor, liquid, or crystal (bilayer ice) phases, depending on the values of pressure (P) and separation between the plates (d). The P-d phase diagrams at $T = 300$ K and $T = 220$ K show that cooling suppresses the vapor phase and stabilizes the liquid and crystal phases. The critical separation $d_c(P)$, below which vapor forms, shifts to lower values of d and P upon cooling. The density profiles show that, upon isobaric cooling or isothermal compression, water approaches the hydrophobic plates. Hence, the effective hydrophobicity of the plate decreases as T decreases and/or P increases, consistent with the observed suppression of the vapor phase. Adding small hydrophilic domains to the hydrophobic plates largely suppresses capillary evaporation and crystallization, highlighting the importance of chemical heterogeneity on hydrophobicity at the nanoscale. Simulations reveal that cooling and/or compression leads to appreciable blurring of the differences between water densities at hydrophobic and hydrophilic surfaces. These observations, together with remarkable similarities in confined water's response to isobaric cooling and to isothermal compression, suggests that the invasion of hydrophobic cavities by water is an important mechanism underlying both pressure and cold denaturation of proteins. Confinement by nominally hydrophobic but chemically-realistic protein surfaces leads to a P-d phase diagram with important differences with respect to the ideal hydrophobic case, with evaporation largely suppressed by the protein's chemical heterogeneity. The compressibility of water confined by protein surfaces is intermediate between that observed in ideally hydrophobic and ideally hydrophilic nano-scale confinement.

Tuesday, February 23 2009 Jonathan Berliner (LIGO Caltech) Laser Interferometer Gravitational Wave Observatory (LIGO)

The LIGO Scientific Collaboration (LSC), a group of hundreds of scientists worldwide, seeks to not only confirm one aspect of Einstein's General Relativity by searching for gravitational waves (GW's) directly, i.e., GW's propagating in space-time, but furthermore, to open the field of gravitational wave astronomy. Though Hulse and Taylor won the Nobel Prize in 1974 for discovering a source of gravitational radiation and Einsteinian Lensing has demonstrated that light curves around massive cosmic objects, the LIGO and Virgo detectors will measure GW's directly. LIGO's interferometers, in Hanford, WA, and in Livingston, LA, are each Michelson interferometers with Fabry-Perot cavities in their 4-kilometer arms, with sensitivities of strain better than 10^{-21} meters per root-Hz. LIGO is also collaborating with the TAROT and Quest telescopes and the Swift Gamma-Ray Burst Mission. NASA and ESA are also planning the Laser Interferometer Space Antenna, to be launched by the end of the decade. This presentation will explore the many challenges and opportunities within the National Science Foundation's most ambitious project ever, including isolating LIGO from terrestrial noises (seismic, thermal, mechanical, metallurgical, atmospheric, anthropogenic), laser/optical noises (shot noise, radiation pressure) and other (digital, electronic, residual gas).

Tuesday, March 2 2009 Relja Vasic (Yeshiva University) Studies of Electronic Structure in Multiferroic Materials

The multiferroics are a significant class of multifunctional materials which show large promise in technological applications such as in electronic, spintronic and memory devices. A hexagonal HoMnO_3 is a model multiferroic material in which ferromagnetic ordering can be switched with an electric field. We have investigated thin film hexagonal and orthorhombic perovskites, HoMnO_3 , and

Y_{0.5}Ho_{0.5}MnO₃ by O K₁ and Mn L_{2,3} edge X-ray absorption spectroscopy (XAS) in normal beam incidence. Thin films were grown by pulsed laser deposition on YSZ(111) and SrTiO₃:Nb (100) substrates which are known to precipitate the hexagonal and orthorhombic phases respectively. The lowest energy XAS features are predominantly Mn 3d states. The MnO₅ and MnO₆ complexes in the hexagonal and orthorhombic films respectively have different symmetries. The electronic structure observed with XAS can be used to distinguish the phases. The XAS spectra on thin films at O K and Mn L edges are useful to determine bonding symmetry and associate features with a molecular orbital model. Preliminary analysis of the XAS spectra have revealed a p-like multiplet structure in the Mn L_{2,3} absorption edge. Further work is focused on angle-resolved resonant photoemission spectroscopy at photon energies at the Mn L_{2,3} edge resonance. The resonance study will be useful to correlate the electronic structure in hexagonal and orthorhombic HoMnO₃ with different types of magnetic order. These spectral features give new insight into the electronic structure of the rare-earth manganate. The results will allow us to develop an understanding of the many-body interactions that play a key role in the electronic structure and functionality of these complex materials.

Tuesday, March 9 2009 Steven Eppell (Case Western Reserve University) Self Assembling Nanophase Composites: A Story of Entropy and Electrostatics

Most man made materials are synthesized by transitioning a high entropy melt to a lower entropy solid. Biological materials break this pattern by condensing a solid phase out of a system whose entropy increases in the process. An additional level of control over how submicron scale structures organize in these systems is obtained by taking advantage of more conventional Coulombic electrostatic interactions. These fundamental physical forces are "manipulated" by controlling the charge and dielectric constants of nanoscale domains on the molecules that assemble to make the material. It will be shown how this balancing act of entropy and electrostatics are used to construct a template for mineralization allowing for a polymer/mineral composite with sub-micron scale phases interdigitated amongst each other. In addition, the resulting mechanical properties of the system at the molecular, supramolecular, and macroscales will be discussed. This is particularly relevant here since the ultimate goal is to produce a load bearing, resorbable, synthetic bone material.

Tuesday, March 23 2009 Mark Edelman (Stern College) Fractional Standard Map

I will present the first results on the basic analysis of the phase space of the fractional standard map (FSM) similar to that done for the standard map of Chirikov. These results are qualitatively new, including new methods, and contain new types of attractors found - slowly converging trajectories, slowly and fast diverging trajectories, attracting ballistic trajectories, and cascade of bifurcation like attracting trajectories. At least one type of fractal-like sticky attractors in the chaotic sea was observed. The Fractional Standard Map is a map with memory and we hope that properties which were found are quite general for all maps with memory. Maps with memory appear not only in physics, but also in finance, in biology, and in social sciences.

Tuesday, April 13 2009 Giancarlo Franzese (University of Barcelona) Slowing Dynamics in Water

Recently, several experiments have investigated the relation between the dynamics of the hydration water and the dynamics of protein. These works have generated a large amount of data whose interpretation is debated. New experiments measure the dynamics of water at low temperature on the surface of proteins, finding a qualitative change (crossover) that might be related to the slowing

down and stop of the protein's activity (protein glass transition), possibly relevant for the safe preservation of organic material at low temperature. To better understand the experimental data several scenarios have been discussed [1]. Here, we review these experiments and discuss their interpretations [2,3] in relation with the anomalous properties [4] of bulk water [5] and confined water [6]. We summarize the results for bulk water and investigate the thermodynamic and dynamic properties of supercooled water at an interface [7]. We will consider also the effect of water on protein stability, making a step in the direction of understanding, by means of Monte Carlo simulations and theoretical calculations, how the interplay of water cooperativity and hydrogen bonds interfacial strengthening affects the protein cold denaturation [8].

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3. M. G. Mazza, K. Stokely, S. E. Pagnotta, F. Bruni, H. E. Stanley, and G. Franzese, Two dynamic crossovers in protein hydration water and their thermodynamic interpretation, arXiv:0907.1810v1 (2009).
4. P. Kumar, G. Franzese, and H. E. Stanley, Predictions of Dynamic Behavior under Pressure for Two Scenarios to Explain Water Anomalies, *Physical Review Letters* 100, 105701 (2008).
5. K. Stokely, M. G. Mazza, H. E. Stanley, and G. Franzese, Effect of hydrogen bond cooperativity on the behavior of water, *Proceedings of the National Academy of Sciences (PNAS)* published online January 8, 2010, doi:10.1073/pnas.0912756107.
6. G. Franzese and F. de los Santos, Dynamically Slow Processes in Supercooled Water Confined Between Hydrophobic Plates, *Journal of Physics: Condensed Matter*, *Journal of Physics: Condensed Matter* 21, 504107 (2009). [7] G. Franzese, A. Hernando-Martinez, P. Kumar, M. G. Mazza, K. Stokely, E. G. Strelakova, F. de los Santos, H. E. Stanley, Phase Transitions and Dynamics in Bulk and Interfacial Water, arXiv:0912.1666 (2009).
7. S. Iskrov and G. Franzese, in preparation.

Monday, April 26 2009 at 12:15 pm 515 Belfer Hall Eduardo Fradkin (U. of Illinois at Urbana-Champaign) Entanglement and Quantum Criticality: Can you hear the shape of Schrödinger's Cat?

The entanglement entropy of a pure quantum state of a bipartite system is defined as the von Neumann entropy of the reduced density matrix obtained by tracing over one of the two parts. Critical ground states of local Hamiltonians in one dimension have an entanglement entropy that diverges logarithmically in the subsystem size, with a universal coefficient that is related to the central charge of the associated conformal field theory. In this colloquium I will discuss the extension of these ideas to two dimensional systems, either at a special quantum critical point or in a topological phase. We find the entanglement entropy for a standard class of $z=2$ quantum critical points in two spatial dimensions with scale invariant ground state wave functions: in addition to a nonuniversal "area law" contribution proportional to the size of the boundary of the region under observation, there is generically a universal finite correction, that is completely determined by the geometry of the partition and the correlations encoded in the critical wavefunction. I will discuss the connection between this universal entanglement entropy and the nature of the topological phase. The

application of these ideas to quantum dimer models and fractional quantum Hall states will be discussed.

Tuesday, May 4 2009 Shekhar Garde (Rensselaer Polytechnic Institute) Hydration of Nanoscale Interfaces: from Water Structure and Fluctuations to Hydrophobicity

Abstract (TBA)

Tuesday, September 8 2009 Armin Bunde (University of Giessen, Germany) The clustering of extreme events in climate and financial records

Abstract (TBA)

Tuesday, September 15 2009 Daniel Prober (Yale University) Ultrasensitive Nanobolometers - Superconducting Single-Photon Detection

Recent experiments at Yale have explored the high frequency response of superconducting nanobolometers that are candidates for detecting single Terahertz (4 meV) photons. We can test these optically with a room-temperature Fourier transform spectrometer. We have developed a new testing method with a new 'quanta', the faux photon, = 'fauxton', that allows the much more difficult device testing at the single photon level, for such low photon energies. Using the Fourier transform spectrometer, we have also studied the electrodynamic response of single-walled carbon nanotubes at THz frequencies, to measure the plasmon dynamics and Luttinger physics.

Tuesday, September 22 2009 Vadim Oganessian (College of Staten Island City University, New York) Energy Transport in Models of Excited Media: Simulations and Surprises

We have studied diffusion of energy through arrays of interacting classical degrees of freedom ("spins") in the presence of frozen disorder. We have focussed on the high temperature regime and tracked evolution of the diffusion constant with disorder strength and found a surprisingly large, several orders of magnitude, change in the former upon only moderate adjustments in the latter. Along with these results we shall also discuss in some detail the physics of many-body localization (which was our motivation), spatial heterogeneities of transport and concomittant chaotic signatures we have observed, as well as some crucial details of our (novel?) numerical procedure that enables a precise study of diffusion.

Tuesday, October 20 2009 Camelia Prodan (New Jersey Institute of Technology) Probing the Membrane Potential of Living Cells by Dielectric Spectroscopy

We present a method to obtain the resting membrane potential from the dielectric behavior of a suspension of living cells by the use of dielectric spectroscopy (DS). The presence of membrane potential has a specific effect on the dielectric behavior of cell suspensions and it can be extracted from the low frequency dielectric dispersion curves. Therefore, we use DS to monitor low frequency dielectric permittivity changes of *E. coli* and mammalian cell suspensions from HEK293-hERG line. For mammalian cells, membrane potential changes are triggered by the use of various pharmaceutical

compounds that act as HERG K⁺ channel blockers and IC₅₀ values (proportionals to the drug potencies) are computed for each compound.

Tuesday, November 10 2009 Linda Reichl (University of Texas at Austin) Quantum Control of Atomic Systems Using Nonlinear Dynamics

Laser radiation interacting with an atomic system can create chaos and non-linear dynamical structures in the phase space of the system. These dynamical structures induce fundamental, but controllable, changes in the quantum dynamics of the atomic system. Using laser radiation it is possible, for example, to stabilize electrons that would otherwise ionize and coherently control internal transitions in atomic systems. We will demonstrate these effects for two very different types of system: the internal dynamics of atomic and molecular systems and the coherent control of clouds of cold atoms.

Tuesday, November 17 2009 Mark Edelman (Yeshiva University) Fractional Standard Map

I will present the first results on the basic analysis of the phase space of the fractional standard map (FSM) similar to that done for the standard map of Chirikov. These results are qualitatively new, including new methods, and contain new types of attractors found - slowly converging trajectories, slowly and fast diverging trajectories, attracting ballistic trajectories, and cascade of bifurcation like attracting trajectories. At least one type of fractal-like sticky attractors in the chaotic sea was observed.

Tuesday, November 24 2009 Onforio Annunziata (Texas Christian University) Multicomponent diffusion in micellar and macromolecular aqueous solutions

Diffusion coefficients are fundamental parameters used for describing mass-transfer processes and probing molecular interactions. Our work focuses on understanding diffusive transport in drug-micelle-water and macromolecule-salt-water ternary systems relevant to controlled-release technologies and phase transitions. Experimentally, we use Rayleigh interferometry to determine the four multicomponent diffusion coefficients required for accurately describing isothermal diffusive transport in ternary systems. This seminar will first describe the effect of both micelle concentration and micelle concentration gradient on the diffusive transport of drug compounds. A model based on drug-micelle binding, counter-ion effects and micelle hydration was developed to explain our measured multicomponent diffusion coefficients. The seminar will then show how multicomponent diffusion coefficients can be utilized to extract thermodynamic preferential-interaction parameters for macromolecule-salt aqueous systems. Our extracted parameters were used to reveal new aspects on the dependence of protein solubility on salt concentration.

Tuesday, December 1 2009 Dietmar Paschek (RPI) Computer Simulation Studies of Protein Denaturation by Urea

The natural environment of proteins in the cell is nothing like the dilute aqueous solution found in a typical test-tube situation. Instead, it is a highly concentrated mixture of macromolecules, salts, as well as small molecules acting as “denaturants” or “protecting agents”, either destabilizing or

stabilizing the native state of proteins. Despite decades of effort, there is still considerable debate on how denaturants such as urea or protecting agents such as TMAO interact with proteins. Atomic detail computer simulations are perhaps the ideal tool to provide insight into the molecular aspects of protein thermodynamics. However, previous studies have been mostly focusing on mechanistic aspects of the unfolding of proteins by analyzing initial parts of single unfolding events. We report for the first time a study on the effect of urea on the folding/unfolding equilibrium of Trp-Cage miniprotein by employing replica exchange molecular dynamics (REMD) simulation techniques. Our simulations favor a “direct mechanism”, caused largely by non-specific interactions of urea with the protein. Here van der Waals and electrostatic interactions are found to stabilize the denatured state to almost equal degree. In addition, complementary studies of the behavior of larger proteins such as lysozyme in concentrated urea solutions suggest the importance of cooperative co-solvent phenomena in the very initial steps of protein denaturation, not reported hitherto.

Tuesday, December 8 2009 Theja N. De Silva (SUNY Binghamton) Title (TBA)
Abstract (TBA)

Tuesday, December 15 2009 Beatriz Roldan Cuenya (University of Central Florida) Atomic Vibrations in Metal Nanostructures

Metallic nanostructures are of great interest in many scientific fields due to their novel size-dependent physical and chemical properties. Intriguing effects such as phonon confinement and phonon localization at interfaces have been observed on low dimensional systems. Such modifications in the vibrational (phonon) density of states (PDOS) of nanoscale materials are of scientific and technological relevance, because they profoundly affect their thermodynamic properties. To study these effects homogeneous and size-selected nanostructures are needed. We have synthesized size- and shape-selected ^{57}Fe , $^{57}\text{Fe}_x\text{Pt}_{1-x}$, and $^{57}\text{Fe}_x\text{Au}_{1-x}$ nanoclusters (NCs) with well defined interparticle distances by means of diblock copolymer encapsulation. The clusters were supported on $\text{TiO}_2(110)$ and $\text{SiO}_2/\text{Si}(111)$. The size- and composition-dependent vibrational dynamics of these clusters as well as of nanostructured metal multilayers was measured by nuclear resonant inelastic X-ray scattering. An enhancement of the density of low- and high-energy phonon modes as well as non-Debye-like behavior was observed on ^{57}Fe clusters. The latter effects were found to depend on the chemical nature of the surface shell on the NCs. Drastic deviations were observed in the PDOS of $^{57}\text{Fe}_x\text{Au}_{1-x}$ and $^{57}\text{Fe}_x\text{Pt}_{1-x}$ NCs with respect to the PDOS of their respective bulk alloys. Nevertheless, the PDOS of fcc $^{57}\text{Fe}_{0.75}\text{Pt}_{0.25}(\text{core})/\text{PtSi}(\text{shell})$ NCs was found to retain features of bulk ordered Fe_3Pt Invar alloys, in particular the transverse-acoustic [110] TA1 mode near 9 meV. Apparently, this mode is not affected by size effects and its presence is a pre-requisite for the persistence of Invar-related effects in Fe_3Pt NCs.

Thickness-dependent phonon confinement effects were detected on nanoscale $^{57}\text{Fe}/\text{M}$ multilayers ($\text{M} = \text{Cu}, \text{Pd}$ or Ag). All of these effects show the unique physical properties of metal nanostructures, and their promise in technological applications.

Tuesday, May 12 2008 Brigita Urbanc (Drexel University) The Role of Computer Simulations in Therapeutic Approaches to Alzheimer's Disease

Alzheimer's disease is the leading cause of dementia in elderly. The major risk factor is age. Due to the rapid aging of the American population the costs of care for the patients are rapidly rising. Exactly what causes the dementia is still unclear. Substantial evidence is implicating one protein, called amyloid β -protein (Ab), which is normally present in the brain but undergoes structural changes that cause its aggregation and result in formation of amyloid (senile) plaques in the brain of Alzheimer's patients. I will describe a computational approach that allows the study of initial events of the assembly of Ab into small assemblies, oligomers, which are believed to be the most toxic assemblies responsible for the onset of the disease. I will then describe how this computational approach can identify potential therapeutic targets and examine effects of peptide inhibitors on Ab oligomer formation, thereby providing key structural information of use in drug development.

Monday, August 25 2008 Margarita Ruda (Centro Atomico Bariloche) Hydrogen storage in metallic nanoclusters

Understanding the process of absorption and desorption of H in metals is important for applications such as the design of new materials apt for safe H storage and the development of catalysts for industrial reactions. Equilibrium properties such as the P-C isotherms that characterize the H absorption are modified when this process takes place in nanoparticles instead of the metallic bulk. These phenomena are related to the higher proportion of surface atoms in nanoparticles compared to bulk materials. By performing atomistic simulations the effect of the size of nanoparticles on the H absorption properties can be assessed. Potentials of the Embedded Atom type (EAM) were used to model the atomic interactions while the Monte Carlo technique in the TPmN ensemble allowed to simulate the P-C isotherms. Related thermodynamic properties were calculated from these isotherms according to van't Hoff's equation. Ni and Pd are examples of metals that absorb H in the octahedral interstitials of their fcc lattice. They form hydrides when all these sites are full. The main difference between them is that Pd is a very strong H absorber while Ni is not. Results for H in Ni and Pd will be presented, both for the bulk and for different-sized nanoparticles. The simulation results are compared to experimental data from the literature when available. The calculations are very sensitive to the selection of the potentials, and for Pd two different sets of EAM potentials show different results in terms of the miscibility gap in the bulk and the segregation of H in nanoparticles.

Tuesday, September 9 2008 Latha Venkataraman (Columbia University) Conductance of single molecules circuits

Understanding the transport characteristics of molecules bonded between metal electrodes is of fundamental importance for molecular scale electronics. It is well known that these transport characteristics are influenced by the intrinsic properties of the molecules, including their length, conformation, the gap between the highest occupied molecular orbital and the lowest unoccupied molecular orbital and the alignment of this gap to the metal Fermi level. This talk will focus on the relation between intrinsic molecular properties and the conductance of single molecule junctions formed by breaking gold point-contacts in an environment of molecules with amine linkages. The relation between molecular conductance and molecule conformation for the simple case of a biphenyl, two benzene rings linked together by a single C-C bond will be presented. Specifically, I will show that for a series of seven biphenyl derivatives, the molecular junction conductance decreases with increasing twist angle, following a cosine squared dependence. I will also show that for substituted benzenes, the conductance varies inversely with the calculated ionization potential of the molecules. This reveals that the occupied states are closest to the gold Fermi energy, indicating

that the tunneling transport through these diamine molecules is analogous to hole tunneling through an insulating film

Tuesday, September 16 2008 David Schmeltzer (City University of New York) The physics of correlated electrons—exact solutions based on Dirac's first and second class constraints

Abstract (TBA)

Tuesday, September 23 2008 George Thurston (Rochester Institute of Technology) Studies of the phase diagram and liquid structure of eye lens protein mixtures

In cataract, the leading cause of blindness worldwide, scattering of light in the lens of the eye degrades vision. One possible source of this light scattering is a phase transition within the eye lens cytoplasm. Concentrated protein mixtures in the lens create a high index of refraction that helps focus light on the retina. However, these mixtures can scatter light and can separate to form coexisting liquid phase droplets that differ in refractive index, and thereby cloud the lens./p>
We are studying the aqueous phase diagram of mixtures of the lens proteins, gamma-B-crystallin and alpha-crystallin using light scattering, X-ray scattering and neutron scattering, simulation and modeling. We have found that concentrated mixtures of gamma-B and alpha can separate reversibly to form two liquid phases at and above body temperature, even though gamma-B alone separates only below $\sim 10^\circ\text{C}$, and alpha alone does not phase separate. The molecular interactions emerging as key to the observed phase separation are: gamma-B-gamma-B attractions that drive liquid-liquid phase separation with an upper consolute point, size disparity between alpha and gamma-B, leading towards compositional phase separation, and net attractive gamma-B-alpha interactions and clustering of gamma-B, both of which mitigate compositional phase separation. The phase boundary locations are quite sensitive to the interaction strengths, as is common for other protein condensation diseases. By combining small-angle neutron scattering, simulation and modeling, we are finding that the stability of concentrated alpha and gamma-B mixtures depends sensitively on gamma-B-alpha attraction in a non-monotonic manner: both stronger and weaker gamma-B-alpha attractions are predicted to result in enhanced instabilities, of differing types.

Tuesday, October 28 2008 Tsampikos Kottos (Wesleyan University) Avalanches of Bose-Einstein condensates in leaking optical lattices

We study the decay of an atomic BEC population $N(\tau)$ from the leaking boundaries of an Optical Lattice (OL). For a rescaled interatomic interaction strength $\lambda > \lambda_b$, self-trapped Discrete Breathers (DB's) are created, preventing the atoms from reaching the leaking boundaries. Collisions of other lattice excitations with the outermost DB's, result in avalanches (jumps) in $N(\tau)$ which for $\lambda_b < \lambda < \lambda_*$ follow a scale free distribution $P(J = \Delta N) \sim 1/J^\alpha$. A theoretical analysis of the mixed phase-space of the system, indicate that $1 < \alpha < 3$ in agreement with our numerical findings. We point out that although our focus is given to atomic BECs, our results are also relevant in a large variety of contexts, most prominently being the light emittance from coupled non-linear optics waveguides.

Tuesday, November 4 2008 John Rehr (Washington University) Dead or alive: the role of dynamic structure at the nano-scale

What is the structure of matter at the nano-scale? This question is at the heart of understanding many fundamental problems in science, ranging from physics and chemistry to catalysis to biology. We show in this talk that the conventional picture in terms of a uniquely determined equilibrium structure no longer holds. That picture provides a direct connection between structure and function: according to the laws of physics, the properties of a system are uniquely determined by its structure. This gives rise to the DIRECT PROBLEM of calculating behavior IF the structure is known. This comes back to the original question: what is the structure? Part I of this talk address this question, which is called the INVERSE PROBLEM [1], and more difficult to solve [1]. The reason is that the inverse problem is mathematically "ill-conditioned." Nevertheless, stable solutions can be obtained using a Bayesian approach based on prior knowledge [2]. Such Bayesian methods are now used in many areas of science, for example in obtaining reliable predictions of climate change. In nano-scale science these techniques are essential, as the description of structure requires more parameters than can be determined by experiment. However, this picture is based on a hidden assumption that a unique equilibrium structure exists.

In part II of this talk we show that this assumption only applies to a "dead," skeletal picture, which fails at the nano-scale. In analogy with Brownian motion, we find that nano-scale structures are never in equilibrium, and can only be described using an "animate," dynamic picture. This new real-time picture turns out to explain the many of the unusual properties of nano-scale catalytic materials [3], and has the potential to explain many hitherto unsolved problems in science.

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2. H.J. Krappe and H. H. Rossner, Phys. Rev. B. 66, 184303 (2002); J. Kozden, J. Kas, H. Krappe, H. Rossner and J.J. Rehr, J. Synchrotron Rad. 12, 70 (2005).
3. J. H. Kang, L. D. Menard, R. G. Nuzzo and A. I. Frenkel, J. Am. Chem. Soc. 128, 12068 (2006); F. Vila, J.J. Rehr, J. Kas, R.G. Nuzzo, A.I. Frenkel, Phys. Rev. B 78, 121404(R), 2008.

Tuesday, November 11 2008 Marcos Rigol (Georgetown University) Is there thermalization in isolated quantum systems?

Time dynamics of isolated many-body quantum systems has long been an elusive subject. Very recently, however, meaningful experimental studies of the problem have finally become possible stimulating theoretical interest as well. Progress in this field is perhaps most urgently needed in the foundations of quantum statistical mechanics. This is so because in generic isolated systems, one expects nonequilibrium dynamics on its own to result in thermalization: a relaxation to states where the values of macroscopic quantities are stationary, universal with respect to widely differing initial conditions, and predictable through the time-tested recipe of statistical mechanics. However, it is not obvious what feature of many-body quantum mechanics makes quantum thermalization possible, in a sense analogous to that in which dynamical chaos makes classical thermalization possible. Underscoring that new rules could apply in this case, some recent studies even suggested that statistical mechanics may give wrong predictions for the outcomes of relaxation in such systems. In this talk we demonstrate that an isolated generic quantum many-body system does in fact relax to a state well-described by the standard statistical mechanical prescription. Moreover, we show that time evolution itself plays a merely auxiliary role in relaxation and that thermalization happens instead at the level of individual eigenstates, as first proposed by J. M. Deutsch and M. Srednicki. A striking

consequence of this eigenstate thermalization scenario is that the knowledge of a single many-body eigenstate suffices to compute thermal averages---any eigenstate in the microcanonical energy window will do, as they all give the same result.

Tuesday, November 18 2008 Ben Ocko (Brookhaven National Laboratory) Surface freezing

Most surfaces, as predicted by simple statistical mechanics arguments, melt at a temperature lower than that of the bulk. In this case, a thin terminal liquid layer coexists with the bulk solid. However, the opposite phenomenon, surface freezing, occurs for chain molecules such as n-alkanes. In these systems the surface freezes at a temperature where the bulk remains molten. A thin crystalline layer, ~2nm thick, terminates the bulk liquid over a narrow range of temperature. In this talk I will review x-ray and surface tension measurements of surface freezing at the liquid/air interface for a variety of different molecular systems and explore the chain length dependence. I will also show recent results that indicate that surface freezing can also happen at liquid/liquid and liquid/solid interfaces.

Tuesday, November 25 2008 Lorna Dougan (Columbia University) Identifying the role of the solvent environment in protein folding using single molecule force spectroscopy

Abstract (TBA)

Tuesday, December 2 2008 Pablo Debenedetti (Princeton University) Water in confined spaces

Abstract (TBA)

Tuesday, December 9 2008 David Vanderbilt (Rutgers University) Theory of electric polarization and orbital magnetization

Electric polarization and orbital magnetization turn out to be surprisingly difficult concepts to define precisely in a quantum-mechanical context, despite the fact that they are central to any elementary treatment of electrostatics and magnetostatics. I will review the theory that has emerged to describe the polarization and magnetization in 1993 and 2005, respectively. The basic approach is to decompose the continuous charge distribution into localized packets, known as Wannier functions, whose contributions are well defined. I will also explain how the theory can alternatively be cast in terms of so-called "Berry phases" and "Berry curvatures" defined in terms of the crystal eigenstates. These two approaches provide complementary but equivalent viewpoints on the physics of electric polarization, orbital magnetization, and related phenomena.

Tuesday, December 16 2008 Abraham Lenhoff (University of Delaware) Crystallization and other adventures on the protein phase diagram

The phase behavior of protein solutions is exploited in numerous applications, such as precipitation and crystallization in protein separations, crystallization in structural biology and gelation in food processing. However, the relation of these operations to the phase diagram is not always clearly defined, and detailed phase diagrams have been measured only sparingly, so the phase diagram per se has found only limited use in seeking optimal process conditions. Probably the closest explicit link between a direct property measurement and selection of process conditions for proteins is a

correlation, developed by George and Wilson, of the osmotic second virial coefficient with solution conditions conducive to crystallization. This presentation will discuss efforts to build on the empirical correlation, including more efficient measurement of protein interactions by self-interaction chromatography, making possible a much more extensive exploration of protein interaction trends as a function of solution conditions than has previously been possible. Molecular mechanics simulations are used to explore the mechanistic basis for sometimes counterintuitive trends in virial coefficient measurements. Such measurements will also be related to protein phase behavior measurements, which are organized within the framework of the theoretical phase diagram for short-ranged colloidal interactions. However, a key feature remains the distinctive and complex nature of protein interactions, which give rise to rich and complex physicochemical phenomena and make life possible.

Tuesday, February 3 2007 James Gunton (Lehigh University) Protein Condensation: Kinetic Pathways to Crystallization and Disease

When a system phase separates into two or more phases, there are typically many possible kinetic pathways to equilibrium. Being able to obtain the desired outcome often requires controlling the pathway the system follows. In this talk we will discuss an interesting example of this, namely, the crystallization of proteins from solution. Scientists are trying to grow high quality proteins from solution, in order to determine their structure by X-ray crystallography. It is important to determine protein structure in order to determine protein function. The crucial bottleneck in the crystallization process is crystal nucleation. As a consequence scientists have been trying to determine the dependence of the phase diagram and crystal nucleation rate on the initial conditions of the solution, which typically consists of proteins, water, salt and buffer. A major theoretical difficulty is the absence of an accurate description of the protein-protein interactions in solution. This talk will review some recent theoretical developments regarding the important role of salts and water on these protein phase transitions.

It is also the case that several human diseases are caused by undesirable protein condensation. In such cases, the goal is to understand the underlying kinetics of these phenomena, in order to slow down or prevent nucleation. We will briefly discuss one important example of sickle cell anemia.

Tuesday, February 10 2007 Andrei Bernevig (Princeton University) High-temperature Superconductivity in Iron-based Superconductors

Recently a series of new iron-based materials have broken the cuprate monopoly on high-temperature superconductivity. Similar to the cuprates, these materials have an antiferromagnetic ground-state, though of a different type (colinear). Unlike the cuprates, they are bad metals, rather than insulators at half filling. I will review several of the established experimental facts in the field and I will also discuss how several apparently contradictory measurements such as penetration depth, arpes and NMR spin relaxation rate could in principle be reconciled by a novel kind of superconducting pairing symmetry. I will argue that the most natural explanation of such a pairing symmetry lies in a strong-coupling theory that takes into account the peculiarities of the underlying atomic structure. Upon doping, the antiferromagnetic interactions naturally give rise to a new pairing symmetry, an extended s-wave of the form $\cos(k_x)\cos(k_y)$ in the Brillouin zone instead of the d-wave form present in the cuprates. This order parameter exhibits sign reversal between the electron and hole pockets of the iron-based superconductors.

Tuesday, February 17 2007 Luis Cruz (Drexel University) Geometry and Organization in the Brain: Possible Connections to Cognition

In normal aging our brain suffers from a progressive loss of function, or cognitive decline, expressed as a gradual deterioration in memory, learning, and concentration. The importance of understanding the mechanisms involved in this decline is growing as an increasingly larger percentage of our population ages. In neurodegenerative disorders like Alzheimer's disease the cause of progressive cognitive impairments is the progressive loss of cortical neurons. In contrast, the cause of the relatively mild cognitive impairments in normal aging remains unclear as cortical neurons are not lost. This seminar addresses the hypothesis that cognitive decline in normal aging results from subtle processes that involve the loss of organization in the neuronal architecture. To test this hypothesis, we analyzed brain tissue from behaviorally tested rhesus monkeys, a model for normal human aging, and specifically examined the microcolumn, a vertical array of interconnected neurons that may constitute a fundamental computational unit in the brain. For this, we developed a neuron recognition method that uses segmentation with active contours and machine learning to locate neuronal positions in digitized montages and designed a density map method to quantify changes in microcolumns. Applying these to the aging monkey, we demonstrated a decrease in the "strength" of microcolumns with age that correlates with some cognitive impairments. To determine the exact changes in neuronal organization, we then applied computer modeling that from two-dimensional images constructs virtual 3D representations of neuronal arrangements. This model demonstrated that the observed changes in microcolumns can be accounted by small random displacements of neuron positions of only a few microns. While the biological mechanisms remain to be determined, this loss of microcolumnar organization strongly implicates neuronal disorganization as an active player in cognitive decline.

Tuesday, February 24 2007 Special Location: 1214 Belfer (also no video connection) Peter Vekilov (University of Houston) Metastable Mesoscopic Phases in Protein Solutions

The Gibbs's definition of a phase assumes completely homogeneous composition, with fluctuations bringing about local variations of less than a few percent. We apply light scattering, atomic force microscopy and other techniques to demonstrate that even solutions of a single protein of moderate concentration do not comply with this definition. In such solutions clusters of sizes from several tens to several hundred nanometers exist and have limited lifetimes. These clusters have a higher free energy than the protein solution, and their lifetime is determined by the barrier for their decay. The clusters are an essential part of protein condensation and aggregation pathways. Cluster theories developed for colloid systems appear inapplicable to proteins due to the high level of implied Coulombic repulsion. We put forth and test that these clusters form via hydration forces between protein molecules, thus explaining the apparent ubiquity of the clusters under a broad range of conditions, and their sensitivity to the chemical composition of the solution. We predict and observe a crossover of cluster relaxation to critical-like density fluctuations at high concentrations, and also a universal scaling law for cluster dynamics with time/wave-vector. We estimate and test the size and size-relaxation times of the clusters, the dependence of the cluster volume fraction on the bulk protein concentration, and their response to external parameters. These findings suggest a physico-chemical pathway for the control of protein aggregation: via the structure of the water shell around the protein molecules in solution.

Thursday, March 5 2007 (Special Club-hour Colloquium) Carlos Condat (Universidad Nacional de Cordoba) Microorganism Locomotion: How Speed-dependent Nutrient Absorption can enhance Bacterial Motility

Marine bacteria often reach high swimming speeds, either to take advantage of evanescent nutrient patches or to beat Brownian forces. Since this implies that a sizable part of their energetic budget must be allocated to motion, it is reasonable to assume that some bacteria are able to increase their nutrient intake by increasing their speed v . We formulate a model that uses the concept of internal energy depot to investigate this hypothesis, postulating that the nutrient absorption rate is of the form $q(v) = q_0 + Av$, with q_0 and A being constants. We find the stationary solutions and analyze their stability and the influence of thermal noise. We also show that the mechanical efficiency of the molecular motors increases with A . The description of the motion is further clarified by the use of a Fokker-Planck formalism. Evaluations carried out using realistic parameter values indicate that the speed increase due to the enhanced nutrient absorption may be substantial.

Tuesday, March 24 2007 Bill Wootters (Williams College) Nonlocality in Quantum States and Quantum Measurements

Entanglement is a characteristically quantum mechanical kind of correlation with no analog in classical physics. In fact Schrödinger argued that entanglement was the one feature of quantum mechanics that forced a departure from the classical paradigm. Since the 1980's, entanglement has also been seen as having technological value; certain quantum cryptographic schemes, for example, are based on entanglement. In this talk I review some of the properties and uses of entangled states, and I discuss a more recently discovered kind of nonlocality: the nonlocality of measurements. Many quantum measurements are "more nonlocal" than the states they aim to distinguish. But it is not yet clear what qualities of a quantum measurement contribute to this additional nonlocality.

Tuesday, March 31 2007 Mark Tuckerman (New York University) Enhanced conformational sampling and free energies via novel spatial-warping transformations and adiabatic dynamics

One of the computational grand challenge problems is to develop methodology capable of sampling conformational equilibria in systems with rough energy landscapes. If met, many important problems, most notably protein structure prediction, could be significantly impacted. In this talk, I will present a new approach in which molecular dynamics is combined with a novel variable transformation designed to warp configuration space in such a way that barriers are reduced and attractive basins stretched. The new method rigorously preserves equilibrium properties while leading to very large enhancements in sampling efficiency. The performance of the method is demonstrated on long polymer chains and simple protein models and is shown to significantly outperform replica-exchange Monte Carlo with only one trajectory. Finally, a new molecular dynamics approach for generating multi-dimensional free-energy surfaces that employs adiabatic dynamics combined with multiple time-step integration to drive a set of extended phase-space variables as a means of enhancing the sampling of a subspace of collective variables will be presented.

Tuesday, April 21 2007 Valeria Molinero (University of Utah) Mono-atomic Model of Water

Water is the most ubiquitous liquid in our planet, yet its properties are far from ordinary. The simple structure of the H₂O disguises a very anomalous behavior of the liquid. The most intriguing water anomaly is the existence of two distinct amorphous solids, with different density and structure. It has been proposed that these two pure water glasses originate different liquid phases, and these may be responsible for water's quirks.

In this presentation I will show that the anomalies and phase behavior of water can be understood in the context of other liquids that form tetrahedral structures: the group IV elements. We find that water behaves as an intermediate element between carbon and silicon, and use this concept to develop a simple model of water with which we study the effect of water polyamorphism on the nucleation of ice. The results of our simulations of bulk and confined water indicate that low-density liquid water is the mother of ice, and that the freezing temperature of water can be predicted from knowledge of the location of the liquid-liquid transition temperature TLL. I will discuss the implications of this relationship for the prediction of ice formation in materials and the distinct case of ice formation in hydrophobic confinement where ice can form above room temperature.

Tuesday, April 28 2007 Eric Akkermans (Yale University) Dicke Superradiance and Anderson Localization of Photons

It is generally accepted that coherent multiple scattering of photons in a gas of randomly distributed atoms leads eventually, for a strong enough disorder, to a localized phase where photons are trapped within the gas for extremely long times. The main characteristics of this zero temperature phase transition named after P.W. Anderson are well known and they will be briefly presented. In an atomic gas, however, there exist cooperative effects which change considerably the photon escape rates and the long range atomic dipolar interactions. The resulting enhanced (superradiance) or decreased (subradiance) emission thus competes with localization effects which are very sensitive to long range correlations between scatterers. The purpose of this talk is to compare the two phenomena and to show that for strong enough disorder, photons become localized but this localization appears as a smooth crossover which is primarily determined by cooperative effects rather than by disorder. This crossover is studied in detail using a universal scaling function whose behavior is obtained both from a microscopic analysis and from a modified stochastic Markov process which shares a lot of similarities with "small world networks" well documented in statistical mechanics.

Tuesday, May 5 2007 Alexander Grosberg (New York University) Statistical Mechanics of Knots in Polymers

The mathematics and physics of knots has a long and fascinating history, starting from a model of an atom suggested by W. Thompson (Lord Kelvin) and enthusiastically supported by Maxwell. Knots in DNA are abundant and important. Recently, we surveyed the protein data bank and found that evolution for some as yet unknown reason strongly preferred unknotted proteins. In theoretical aspect, the field was long dominated by either highly abstract mathematics or computer simulations. Recently, some progress was made in the direction of physical understanding of knots. One fruit of it is the prediction that knots under certain circumstances behave like a material with negative Poisson ratio. In the talk, all these various aspects will be reviewed in some mixture.