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 ligh-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 Bernouill'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.

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-

November 13th

Mikhail Anisimov
Institute for Physical Science and Technology
Departmenr of Chemical and Biomelcular Engineering, University of Maryland, College Park

Entropy-Driven Liquid-

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

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

also take place

P797.95 Tm[( )] TJET1 g70.58ETBT1 0 0 1 335.11 511.15 Tm[( )] TJ1EBT1 0 0 1 4P797.95 Tm[( )] TJET1 g70.5834ETBT1 0 0 1

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:

Re 454.27 Tm[( )] TJET 1 62 TJET2.,

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

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.

Sequential Behavior in Dynamical Networks

Abstract:

Dynamical networks are mathematical models that describe an activity of biological, cognitive and other real systems. They consists of active elements possessing their own dynamics joint

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 until the 1850s that instruments could recognize a tenth of a second, and, once they did, the impact on modern science and society was

modules.

December 6th

Hugo Fort

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

October 4th

Francesca Tria
ISIF, Torino, Italy

of homogeneous and heterogeneous catalysts are studied during their synthesis and activity, with a combination of complementary

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-

Furthermore to understand the soft-mode driven oxygen diffusion phenomenon we analyzed the counterpart system CaFeO2.5, 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, litation technologies are inadequate. In severe brainstem stroke and advanced ALS, both the ability to speak - 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 dc(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

Y.5Ho.5MnO3 by O K1 and Mn L2,3 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

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].

1. "Aspects of hysical Biology Biological Water, Protein Solutions, Transport and Replication", Book Series: Lecture Notes in Physics , Vol. 752/2008, G. Franzese and M. Rubi (Eds.), Springer Berlin 2008, 280 p.
2. G. Franzese, K. Stokely, X.-Q. Chu, P. Kumar, M. G. Mazza, S.-H. Chen, and H. E. Stanley,

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) Hydra

compounds that act as HERG K+ channel blockers and IC50 values (proportionals to the drug pottencies) 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 a

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

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 b-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 assesed. Potentials of the Embedded Atom type (EAM) were used to model the atomic interactions while the Monte Carlo technique in the TPmN ensamble allowed to simulate the P-C isotherms. Related thermodynamic properties were calculated from these isotherms

octahedralinterstitials 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

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

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 my simple statistical mechanics arguments, melt at temperature lower

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 s-3( )] TJETh 537.372.024 550.9 -3(s)550.9p2(dar[(na)-3(t)10(e)-3(s)-3(i)3(t)-23(t)-3(w) -2(o)1)7(3)-2(or)

natwa0(e)-3(y)-3(s)4(t)-2e(nc)qo builirim eingebl t

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

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