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Monday, March 10, 2008 8:00AM - 11:00AM –
Session A8 DFD: Colloidal Self-Assembly I Morial Convention Center RO6

8:00AM A8.00001 Directed Self-Assembly of Spherical Particles NATALIE ARKUS, GUANGNAN MENG, VINOTHAN MANOHARAN, MICHAEL BRENNER, Harvard University —

We examine the kinetics and energetics of self-assembly in systems containing a small number of spherical colloidal nanoparticles using a combination of theory, simulation, and experiment. We then explore how the addition of spherically symmetric binding specificity can be used to direct the self-assembly of a given structure.

Using graph theoretic, numerical, and algebraic geometric techniques, we denumerate all possible packings for a system of n particles. We map out the energy landscape of these packings, which is determined not only by the value of the potential energy at these minima, but also by the vibrational normal modes of the structures. Experiments for a 6 particle system show that the likelihood of a given packing follows this expected equilibrium distribution.

To explore the kinetics of packing formation, we simulate the self-assembly of these systems in the irreversible binding limit. For the 6 particle system, this reveals that the kinetics required to form one of the packings is highly unlikely, resulting in the other packing forming with 100% probability. With the addition of binding specificity however, we can cause the unlikely packing to form with 100% probability. We show how the addition of binding specificity effects the energetic landscape of these systems, and that it alone is sufficient to direct self-assembly.

8:12AM A8.00002 Controlling assembly of micro- and nano-particle systems with DNA. , DMYTRO NYKYPANCHUK, MATHEW MAYE, DANIEL VAN DER LELIE, OLEG GANG, Brookhaven National Laboratory — Addressable biological interactions provide attractive platform for rational self-assembly, however the strength of such interactions are often difficult to control. Here we present an approach where DNA molecules are used to balance attractive and repulsive interactions during particles assembly while preserving the interaction addressability. We show, that by changing the composition and structure of DNA shall of micro- (2 um) or nanoparticles (10 nm), assembly kinetics, aggregate sizes, and the systems melting properties can be tuned. At constant environmental conditions, this strategy allows for rational control of interaction energy landscape for nano- and micro-systems in a wide dynamic range.

8:24AM A8.00003 Evaporation-Driven Assembly of Microspheres with Polymer in Emulsion Droplets[1] , KENG-HUI LIN, Institute of Physics, Academia Sinica, Taipei, Taiwan, LIANG-JIE LAI, Dept. of Physics, National Central University, Chung-li, Taiwan, CHIH-CHUNG CHANG, HUI CHEN, Dept. of Chemical and Materials Engineering, National Central University, Chung-li, Taiwan — We study the packing of colloidal microspheres mixed with polymer in oil-in-water emulsion droplets through evaporation. The addition of polymer produce non-unique configurations of final clusters when the number of particles N inside the droplet is larger than 4. The cluster configurations are classified into three categories based on the symmetry. Stablized colloidal clusters of spherical packings are observed. Observation on packing process shed light to the mechanisms which cause different and non-unique structures. The osmotic pressure and interparticle interaction due to polymer play important roles in packing.

[1]Support for this work is provided by NSC Grant No. 96-2112-M-001

8:36AM A8.00004 Entropy-driven self-assembly of dimers , ISSEI NAKAMURA, AN-CHANG SHI, McMaster University — Supramolecular self-assembly is an important phenomenon with applications ranging from chemical synthesis to biological systems. Although the driving force of assembly is the weak non-covalent intermolecular interaction such as hydrogen bonding and dispersion force, the self-assembly is a result from balancing the enthalpic and entropic contributions. In general, the disassembled/disordered phase is expected as temperature is raised because of the entropic gain from the components of the aggregate. However, it has been observed that the self-assembled/ordered phase can be promoted with increasing temperature. This implies that the self-assembly is driven by entropy. In order to provide a better understanding of this entropy-driven transition, we have studied a statistical mechanical model for the aggregation of macromolecular dimers immersed in solvents. The model demonstrates that solvent molecules absorbed on the surface of the solute are released with increasing temperature, leading to an increase of the total entropy of the system. Consequently, the cooperative stability of the dimeric state is induced. The thermodynamic features of this transition are analyzed.

8:48AM A8.00005 Hydrodynamic interactions effects on the dipole-induced self-assembly of β-peptides and Brownian-induced polymer pore translocation , JUAN HERNANDEZ-ORTIZ, Departamento de Materiales, Universidad Nacional de Colombia, Sede Medellin, MICHAEL GRAHAM, JUAN DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — A novel method that scales linearly with the number of particles is used to study Brownian-systems considering fluctuating hydrodynamic interactions. The method is demostrated in the concept of two applications: the dipole-induced self-assembly of β-peptides and the Brownian-motion-induced translocation of a polymer thought a rectangular pore. The method includes the long-range interactions by the Green's function formalism. It allows the consideration of peptides at intermediate concentrations and the inclusion of the non-periodic domain of the translocation. The hydrodynamics interactions affect the dynamics of the peptides agglomeration and the mean-squared-displacement indicates significant changes in the long-time diffusion coefficient. The polymer translocation is study using a transition path sampling based methodology. In particular it is used to calculate the translocation rate constant. Even for a single bead there are differences once hydrodynamics are included. These differences are due to the changes of mobility near walls and the change in polymer chain diffusion coefficient.

9:00AM A8.00006 Self-assembly of complex shaped colloidal particles , ADELINE PERRO, VINOTHAN N. MANOHARAN, Harvard School of Engineering and Applied Sciences — We have developed a new method to produce hybrid particles with polyhedral shapes in very high yield (liter quantities at up to 75% purity) using a combination of emulsion polymerization and inorganic surface chemistry. The optical properties of these particles are tailored for studying their dynamics and self-assembly. For example, we produce systems that consist of index-matched sphere doublets with a small strongly scattering inorganic core between the two spheres, allowing us to track the center of mass of each doublet. We have generalized the preparation procedure to create even more complex geometries, including hybrid tetrahedra and octahedra. We present some preliminary studies on the self-assembly of these systems based on various optical experiments, including confocal microscopy, light scattering, and digital holographic microscopy.

9:12AM A8.00007 Progress on systems of DNA modified colloidal particles for self-replication , PAUL CHAIKIN, MIRJAM LEUNISSEN, REMI DREYFUS, ROUJIE SHA, NADRIAN SEEMAN, DAVID GRIER, DAVID PINE, New York University — Our goal is to create new materials that can self-replicate and self-assemble. For this, we modify the interactions between micrometer-sized colloids by coating them with single-stranded DNA 'sticky ends', which specifically recognize complementary sequences on other colloids. We find that the aggregation-dissociation behavior is fully reversible for at least tens of temperature cycles. Using magnetic beads or optical tweezers, we form a chain-like 'seed' structure, which acts as a template to assemble copies of itself from a soup of singlets. To determine what are the preferred binding sites, we studied the interactions between the singlets and their complementary particles in the seed. Important in our replication scheme is that each particle has two different types of sticky ends: one for 'longitudinal' bonding along the chain and another for 'transverse' bonding between seed and daughter chains. Contrary to the transverse linkers, the longitudinal linkers form AT/TA bonds, which can be crosslinked with an intercalator and UV irradiation. In this way, we permanently fix the seed and its copies.

9:24AM A8.00008 Binary Colloidal Assembly by Dielectrophoresis , PETER HOFFMAN, YINGXI ELAINE ZHU, University of Notre Dame — Dielectrophoresis (DEP)-driven colloidal assembly has been recently explored as a new route to manipulate colloids and rapidly form nanostructured materials. In this talk, we demonstrate that colloidal particles of varied sizes can be assembled with controllable packing configurations in the presence of AC-electrical fields. We investigate binary latex particles of varied size ratios from 0.25 to 0.8 and directly monitor the dynamic assembly process with final structural characterization by using high-speed confocal microscopy. We observe rich phase behaviors of binary colloidal assembly with a strong dependence of applied AC-field frequency and medium conductivity. The obtained structural phase diagram can be well predicted by the DEP mobility and the Peclet number. We also present a mechanism that underlies the colloidal charge polarization due to charge segregation and entrainment within the double layer at several distinct frequencies, which cannot be explained by the classical Maxwell-Wagner theory. We recently also employ the same mechanism to form binary colloidal crystals.

9:36AM A8.00009 Unusual aggregation behavior of colloids coated with palindromic DNA , MIRJAM LEUNISSEN, REMI DREYFUS, DAVID PINE, PAUL CHAIKIN, New York University — Coating particles with single-stranded DNA 'sticky ends' gives excellent control over the specificity, strength and range of their interactions. Usually, a pair of complementary 'Watson-Crick' sequences is used to obtain thermoreversible binding of different colloids. However, for certain purposes one could also use self-complementary 'palindrome' sequences. Using light microscopy, we studied the aggregation behavior of micrometer-sized palindrome-coated colloids. Unlike Watson-Crick sticky ends, we found that it is of great importance whether the palindrome sticky end is attached to a flexible single strand or a rigid double-stranded 'rod'. While the latter system displayed normal dissociation at elevated temperature, the former system showed enhanced aggregation with increasing temperature and no aggregation during fast temperature quenches. We explain these unusual observations by a competition between intra- and interparticle bonds. This provides us with an additional level of control over the interparticle bonding, besides the sequence of the sticky ends, the salt concentration and the DNA density on the beads.

9:48AM A8.00010 Functionalized Au nanoparticles in solution , GARY S. GREST, J. MATTHEW D. LANE, Sandia National Labs — The properties of functionalized Au nanoparticles in decane and water were studied by large-scale explicit atom, molecular dynamics simulations. Gold nanoparticles functionalized with S-$(CH_2)_9$-X alkanethiols chains (X = COOH or CH_3) were studied at the liquid-vapor interface and in the bulk. The structure of the functional groups on the nanoparticle was found to depend strongly on the end group and solvent. At the interface methyl terminated nanoparticles repel the water and move toward the vapor while in decane, the decane molecules engulf the nanoparticle. In the bulk, results for the nanoparticle/nanoparticle pair correlation function and nanoparticle diffusion will be presented as a function of nanoparticle concentration. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04- 94AL85000.

10:00AM A8.00011 DNA-Grafted Janus Particles , CHING HSUEH, Department of Physics, National Central University, Chungli, Taiwan, KENG-HUI LIN, WEN-TAU JUAN, Institute of Physics, Academia Sinica, Taipei, Taiwan — Recently there have been advances in generating Janus microspheres whose two hemispheres have different chemical compositions [1-4]. The new types of particles open up possibilities for assembly of complex structures. Here we attach DNA molecules onto one side of Janus microspheres. The new type of colloidal particles resembles surfactant molecules and may give us interesting new structures.
Reference: [1] Y. Lu, H. Xiong, X. Jiang, Y.Xia, M. Prentiss and G. M.Whitesides, J. Am. Chem. Soc. **125**, 12724 (2003) [2] O.Cayre, V. N.Paunov and O. D. Velev, J. Mater. Chem. **13**, 2445 (2003) [3] R. F. Shepherd, J. C. Conrad, S. K. Rhodes, D. R. Link, M. Marquez, D. A. Weitz and J. A. Lewis, Langmuir **22**, 8618 (2006) [4] L. Hong, S. Jiang and S. Granick, Langmuir **22**, 9495 (2006)

10:12AM A8.00012 The importance of repulsion in the aggregation-dissociation behavior of DNA coated colloids , REMI DREYFUS, MIRJAM LEUNISSEN, ROUJIE SHA, NADRIAN SEEMAN, DAVID GRIER, DAVID PINE, PAUL CHAIKIN, New York University — Coating particles with DNA gives excellent control over the specificity, strength and range of their interactions. In our experiments, a pair of complementary 'Watson-Crick' sequences is used to obtain thermoreversible binding of different colloids. Colloids coated with such complementary 'sticky' DNA aggregate when they are mixed together, the aggregates dissolve again when they are heated. We investigate the melting behavior of colloids coated with both sticky and non-sticky DNA. By changing the ratio between the sticky and non-sticky DNA, the obtained melting curves have very different melting temperatures, but almost the same sharpness. We show that the sharpness does not change because a high number of bonds bridges the particles, and that the strong shift in melting temperature is due to a repulsive interaction induced by the confinement of the non-sticky DNA when the particles come close together.

10:24AM A8.00013 Self Assembly of Colloidal Particles at Small N , GUANGNAN MENG, NATALIE ARKUS, RYAN MCGORTY, MICHAEL BRENNER, VINOTHAN MANOHARAN, Harvard University — We confine a small number ($N \approx 10$) of micron-sized colloidal particles within micro-wells, and we use this finite system to study the process of self-assembly. The reversible aggregation of colloidal particles is controlled by a short-range depletion attraction, which is induced by poly(N-isopropylacrylamide) nano particles. We use digital holographic microscopy to monitor the structural and kinetic properties of self-assembled colloidal clusters, and we use micro-wells to collect ensemble statistics. We compare our experimental results with theory and simulations, which probe how energetics and kinetics affect the packing structures.

10:36AM A8.00014 2D crystals of Janus amphiphilic colloidal spheres , SHAN JIANG, STEPHEN ANTHONY, University of Illinois at Urbana-Champaign, ANGELO CACCIUTO, Columbia University, ERIK LUIJTEN, STEVE GRANICK, University of Illinois at Urbana-Champaign — Colloidal spheres with one side hydrophilic and the other side hydrophobic assemble into 2D crystals with hexagonal translational order complemented by a high degree of orientational organization. Factors that determine the crystal structure are investigated, especially the dependence on ionic strength and on Janus balance. Depending on these variables, patches of the orientational order can be altered: from doublets to extended lines containing dozens of particles. Janus particles with different geometry (Janus balance) self-assemble into different cluster structures. Collective motion is evident from time-resolved optical microscopy.

10:48AM A8.00015 Harnessing Elastic Instability for the self-assembly of complex patterns , ELISABETTA MATSUMOTO, YING ZHANG, ANNA PETER, PEI-CHUN LIN, RANDALL KAMIEN, SHU YANG[1], University of Pennsylvania — Directed pattern formation through the self-assembly of complex polymer systems promises to be a powerful approach in the pursuit of novel, transformative technologies. Current approaches to create desired motifs at the nanoscale utilize flow, shear, fields, and other externally imposed, top-down forces. Nature, on the other hand, provides us with a plethora of examples of intrinsic, bottom-up effects: from the phyllotactic growth of plants to animal stripes to fingerprints, instabilities, packing constraints, and simple geometries can drive the formation of delicate, detailed, and beautiful patterns. By harnessing the elastic instability in flexible poly(dimethylsiloxane) (PDMS) membranes with a square lattice of circular pores exposed to a solvent, we distort the pores into a pattern featuring long-range orientational order. Within linear elasticity theory, we find the groundstate configuration of a lattice of interacting deformation elements, or "dislocation dipoles" to be in complete agreement with the observed pattern. Our theory allows us a means to design the patterns formed by such elastic frustration.

[1]Department of Materials Science and Engineering

Monday, March 10, 2008 8:00AM - 11:00AM –

Session A9 DFD DBP: Focus Session: Fluid Dynamics of Animal Motion Morial Convention Center RO7

8:00AM A9.00001 Comparing flight strategies in species of fruit flies , ITAI COHEN, LEIF RISTROPH, GORDON BERMAN, Cornell University, Z. JANE WANG, Cornell Univeristy — Observing different species of fruit flies offers an opportunity to compare flight strategies for insects of varying size but of nearly identical body and wing architecture. Using automated three-dimensional high-speed videography, we have captured many beautiful flight sequences of untethered fruit flies. From this data we have extracted the complete body and wing kinematics and determined the fluid forces acting on the wings using custom-written tracking and analysis software. We find that, in addition to lift, drag plays an important role in providing the vertical force needed for these insects to stay aloft. Moreover, our data base in combination with various numerical analysis techniques is allowing us to resolve whether these insects are flapping in the most efficient manner possible. Answers to this line of questions are important for determining what role if any evolution has played in determining how these insect fly.

8:12AM A9.00002 Flow-induced attraction of swimming microorganisms by surfaces , ERIC LAUGA, University of California, San Diego, ALLISON BERKE, MIT, LINDA TURNER, HOWARD BERG, Rowland Institute and Harvard University — In this talk, we present an experimental and theoretical investigation of the accumulation of swimming cells by nearby surfaces. First, we present results of an experiment aiming at measuring the distribution of smooth-swimming E. coli when moving in a density-matched fluid and between two glass plates; the distribution for the bacteria concentration is found to peak near the glass plates. We then present a physical model for the observed attraction, based on the hydrodynamics interactions between the swimming cells and the walls. We show that such interactions result in a reorientation of the cells in the direction parallel to the surfaces, and an attraction of these (parallel) cells by the nearest wall. Our results are exploited to obtain an estimate of the propulsive force of smooth-swimming E. coli.

8:24AM A9.00003 Effects of hydrodynamic interactions in bacterial swimming.[1] , SUDDHASHIL CHATTOPADHYAY, XIAO LUN WU, University of Pittsburgh — The lack of precise experimental data has prevented the investigation of the effects of long range hydrodynamic interactions in bacterial swimming. We perform measurements on various strains of bacteria with the aid of optical tweezers to shed light on this aspect of bacterial motility. Geometrical parameters recorded by fluorescence microscopy are used with theories which model flagella propulsion (Resistive force theory & Lighthill's formulation which includes long range interactions). Comparison of the predictions of these theories with experimental data, observed directly from swimming bacterium, led to the conclusion that while long range inetractions were important for single polar flagellated strains (Vibrio Alginolyticus & Caulobacter Crescentus), local force theory was adequate to describe the swimming of multi-flagellated Esherichia Coli. We performed additional measurements on E. Coli minicells (miniature cells with single polar flagellum) to try and determine the cause of this apparent effect of shielding of long range interactions in multiple flagellated bacteria.

[1]This work was funded by NSF grant #0646573.

8:36AM A9.00004 Lagrangian studies of animal swimming and aquatic predator-prey interactions[1] , JOHN DABIRI, California Institute of Technology — Experimental studies of animal swimming have been traditionally based on an Eulerian perspective in which the time-dependent flow field surrounding the animal is measured at fixed locations in space. The measured velocity field and its derivatives (e.g. vorticity) can, in principle, be used to deduce the forces, energetics, and fluid transport associated with locomotion in real fluids. However, achieving a connection between measurements of these Eulerian fields and the dynamics of locomotion has proven difficult in practice. We present the application of Lagrangian methods of flow analysis in which the time-dependent trajectories of individual tracer particles in the flow are measured experimentally and subsequently interrogated using dynamical systems tools in order to quantitatively resolve the dynamics of animal swimming. The Lagrangian methods are shown to be readily extended to time-dependent measurements in three spatial dimensions and to in situ field measurements using a recently developed self-contained underwater velocimetry apparatus (SCUVA). Case studies of jellyfish and other aquatic animals observed in the laboratory and in marine environments are used to illustrate the proposed approach. We also show that predator-prey interactions during jellyfish swimming can be addressed using the aforementioned Lagrangian methods in combination with the Maxey-Riley equations for inertial particles in fluid flow.

[1]Research supported by NSF Ocean Sciences and Energy for Sustainability

9:12AM A9.00005 Shape transformations and propulsion due to an elastic filament rotating in a viscous fluid , BIAN QIAN, THOMAS POWERS, KENNETH BREUER, Brown University — The deformation of an elastic filament in a viscous liquid is central to the mechanics of motility in cells ranging from *E. coli* to sperm. We use experiments and theory to study the shape transition of a flexible rod rotating in a viscous fluid and set at an angle to the axis of rotation. In the experiments, two modes of operation are studied: constant torque and constant speed, and the shape of the filament is measured using stereoscopic imaging. At low applied torque, the rod bends gently, while at high torque, the rod adopts a helical shape with the tip close to the axis of rotation. At constant torque, the transition from the splayed form to the helical form is abrupt, accompanied by a sharp increase in the rotational speed. As the torque is decreased, the shape change exhibits hysteresis, transitioning back to the splayed form at a lower torque. At constant speed, the shape transition is continuous characterized by a region of decreasing torque that persists until the transition to the helical form is complete. Calculations based on slender body and resistive force theory predict the torque-speed relationship and the filament shape throughout the entire operating range, and show excellent agreement with the experiments. The propulsive force is predicted to increase sharply after the shape transformation, at which point the efficiency is also predicted to reach a maximum.

9:24AM A9.00006 Propulsion by directional adhesion , JOHN BUSH, MANU PRAKASH, MIT — The rough, hairy integument of water-walking arthropods is well known to be responsible for their water-repellency; we here consider its additional propulsive role. We demonstrate that the tilted flexible leg hairs of water-walking arthropods render the leg cuticle directionally anisotropic: contact lines advance most readily towards the leg tips. The dynamical role of the resulting unidirectional adhesion is explored, and yields new insight into the manner in which water-walking arthropods generate thrust, glide and leap from the free surface. We thus provide new rationale for the fundamental topological difference in the roughness on plants and insects, and suggest novel directions for biomimetic design of smart, hydrophobic surfaces.

9:36AM A9.00007 The role of the ventral pedal waves in the locomotion of terrestrial gastropods , JANICE LAI, ROBERT D. SHEPHERD, JUAN C. DEL ALAMO[1], JAVIER RODRIGUEZ-RODRIGUEZ, JUAN C. LASHERAS, University of California San Diego — The locomotion of terrestrial gastropods exhibits unique characteristics which allow these animals to crawl on steep surfaces. Gastropods move by gliding over a ventral foot lubricated by mucus. They generate trains of pedal waves through periodic muscle contractions in the central portion of the ventral foot, producing a forward traction, while the rim of the foot adheres to the substrate and generates suction forces. We analyzed the kinematics and dynamics of locomotion by conducting two sets of experiments. In the first set, we used digital image processing to correlate the frequency and wavelength of the pedal waves to the migration velocity. In the second set, we computed the traction and adhesion forces produced by these animals from measurements of the deformation of an elastic substrate of known properties. We found that the strain energy exerted by the animal on the substrate is quasi-periodic, and explored a possible correlation between the mean speed of migration and the period of this energy fluctuation. In addition, we found that the pedal waves accelerate as they move forward along the ventral foot producing the symmetry break necessary for the generation of a net traction force.

[1]Partially supported by Spanish MEC (Fulbright Program)

9:48AM A9.00008 Flying, swimming and fluttering in 3D: potential flow around a rectangular deformable plate[1] , CHRISTOPHE ELOY, LIONEL SCHOUVEILER, IRPHE, Marseille, France — The interaction between a flexible rectangular plate and the flow around it can serve as a model for several phenomena. This situation arises in many problems of animal locomotion as well as industrial ones such as airfoil flutter. So far, most models have assumed a 2D problem for the sake of simplicity. We show here how to extend these models to include the finite plate aspect ratio in the analysis. We consider a rectangular deformable plate moving in a uniform flow at small amplitude such that the plate and its wake remain in the same plane at first order. The potential flow around the plate is calculated in the Fourier space and then averaged along the span. The result is a new integral equation for the vorticity distribution both inside the solid plate and in its wake. It means that the 3D effects can be taken into account by simply modifying the potential of a point-vortex (or equivalently the Green function of the Laplace's equation).

[1]This work received financial support from the French ANR project DRAPEAU.

10:00AM A9.00009 Symmetry breaking in gastropod locomotion through acceleration or deceleration of the pedal waves , JUAN C. DEL ALAMO[1], JAVIER RODRIGUEZ-RODRIGUEZ, JANICE LAI, ROBERT D. SHEPHERD, JUAN C. LASHERAS, University of California San Diego — Marine and terrestrial gastropods move by gliding over a ventral foot that is lubricated by secreted mucus (terrestrial) or simply by water (marine). The rim of the ventral foot generates suction forces that keep the animal adhered to the substrate. The central part of the foot produces a forward traction force by generating trains of pedal waves through periodic muscle contractions. Recent experiments show that, in some gastropods, these pedal waves become faster and longer as they move forward, suggesting a mechanism for breaking the symmetry in the flow between the pedal waves and the substrate. To investigate this mechanism, we have analyzed theoretically a two-dimensional lubrication layer between a train of waves of slowly varying length and speed, and a flat, rigid, impermeable surface. The inhomogeneity of the pedal waves has been modeled through multiple-scale asymptotics. We have considered a Newtonian fluid to separate the effect of this inhomogeneity from the viscoelastic symmetry breaking reported in previous works.

[1]Partially supported by Spanish MEC (Fulbright Program)

10:12AM A9.00010 The unsteady flow over a bat wing in mid-downstroke. , FLORIAN MUIJRES, CHRISTOFFER JOHANSSON, RYAN BARFIELD, MARTA WOLF, Lund University, GEOFFREY SPEDDING, University of Southern California, ANDERS HEDENSTROM, Lund University — Birds, bats and insects have provided inspiration for human-designed small-scale flying machines, and while insects have long been known to rely on unsteady separated flows for their above-average aerodynamic performance at small-scale, the details of air flows over bird and bat wings have been harder to elucidate, mainly because of the extra complexity and precautions required in live experiments. Here we report on the first experiments of the airflow around a bat wing in free (but trained) flight in a low-turbulence wind tunnel. The aerodynamics of fixed wings at these Reynolds numbers are notoriously sensitive to small disturbances of the initially laminar, attached boundary layer, but these flight experiments show that the instantaneous flow fields around the flapping wing bear almost no resemblance to an equivalent fixed-wing experiment. The circulation increment due to the presence of a strong leading-edge vortex is estimated to provide a significant fraction of the total lift. Implications for the design and control of micro-air vehicles are considered.

10:24AM A9.00011 Mechanics of Mammalian Swimming , TIMOTHY WEI, PAUL LEGAC, Rensselaer Polytechnic Institute, FRANK FISH, West Chester University, TERRIE WILLIAMS, University of California - Santa Cruz, RUSSELL MARK, USA Swimming, SEAN HUTCHISON, King Aquatics — Propulsion of large mammals ($i.e.$ dolphins and humans) has been of great interest for both technological and athletic reasons. The foundational question is how fast can a mammal swim? Digital Particle Image Velocimetry (DPIV) has been modified to be safely used on swimmers and dolphins. Experiments of dolphins performing various swimming behaviors were performed at the Long Marine Laboratory, University of California, Santa Cruz. Vortices generated by the dolphins' tail motions were used to estimate thrust production. Also, a two-dimensional dynamic force balance was constructed to study and improve the mechanics of elite swimmers. Paired with an underwater video camera, the forces seen could be directly related to the motion of the swimmer. These force measurements could be correlated to time resolved DPIV measurements of flow around the swimmers. Measurements made with swimmers, Megan Jendrick (2000 Olympic gold medalist) and Ariana Kukors (4x US National Champion), as well as data from trials with two dolphins will be presented.

10:36AM A9.00012 Synchronization and hydrodynamic interactions , THOMAS POWERS, BIAN QIAN, KENNETH BREUER, Division of Engineering, Brown University — Cilia and flagella commonly beat in a coordinated manner. Examples include the flagella that Volvox colonies use to move, the cilia that sweep foreign particles up out of the human airway, and the nodal cilia that set up the flow that determines the left-right axis in developing vertebrate embryos. In this talk we present an experimental study of how hydrodynamic interactions can lead to coordination in a simple idealized system: two nearby paddles driven with fixed torques in a highly viscous fluid. The paddles attain a synchronized state in which they rotate together with a phase difference of 90 degrees. We discuss how synchronization depends on system parameters and present numerical calculations using the method of regularized stokeslets.

10:48AM A9.00013 An experimental and numerical study of fluid flow generated by a single nodal cilium , XINGZHOU YANG, Center for Computational Science, Tulane University, LISA FAUCI, Department of Mathematics, Tulane University, ARSHAD KUDROLLI, Department of Physics, Clark University — A rotating nodal cilia is said to generate fluid flow in the node of a developing embryo by posterior tilt leading to the left-right asymmetry of the mammalian body. In order to develop a physical understanding of the flow generated and the effect of the enclosing chamber, we perform scaled-up fluid-mechanics experiments and numerical simulations using the method of Regularized Stokeslets for zero Reynolds number. Important mechanical parameters, such as the geometry of the rods, dimensions of the tank, and the ratio of viscous to elastic stresses can be scaled to match typical cilia and cell. Digital imaging and tracer particle tracking techniques are used to measure the location and shape of the rods and the fluid flow. We will discuss the nature of the hydrodynamic velocity fields which are found to be more complex than anticipated by previous studies.

Monday, March 10, 2008 11:15AM - 2:15PM –
Session B8 DFD: Colloidal Self-Assembly II Morial Convention Center RO6

11:15AM B8.00001 Orthogonal Tracking Microscopy for Nanofabrication Research , MATTHEW MCMAHON, ANDREW BERGLUND, PETER CARMICHAEL, JABEZ MCCLELLAND, J. ALEXANDER LIDDLE, National Institute of Standards and Technology — Constructing 2D lateral particle trajectories from digital video sequences of nanoparticle motion in a liquid is straightforward and fairly common, requiring only the use of centroid-finding algorithms. On the other hand, extracting particle trajectories in the third (out-of-plane) dimension has been more difficult, requiring detailed calibration of the radius of the defocused diffracted rings which result from vertical fluctuations of particle position. We introduce a new technique, termed orthogonal tracking microscopy or orthogonal projection microscopy, in which integrated micromirrors produce one or more reflected images of a particle within the same field of view as the direct image. The reflected images project vertical motion into lateral motion. Thus, we are able to construct a fully 3D particle trajectory from 2D digital video using only centroid-finding algorithms. We use this technique to study particle-surface interactions relevant to directed assembly of nanoparticles.

11:27AM B8.00002 Self-Assembly of Colloidal Membranes , EDWARD BARRY, ZVONIMIR DOGIC, Brandeis University — Symmetric monolayer membranes are observed to self-assemble in a colloidal suspension of hard rods with soft attractions. This attractive component to the interaction is enough to drive the self-assembly of stable two dimensional fluid-like surfaces of rods. Simultaneous measurements are made at both the molecular, via direct imaging of individual fluorescently labeled particles, and the continuum length scales. At the continuum scale, the elastic Hamiltonian for a two dimensional fluid-like surface is verified for a symmetric monolayer, and measured material constants such as the bending modulus and the area compression modulus are demonstrated to obey a simple elastic relationship.

11:39AM B8.00003 Self-Assembled 3D Ordered Macroporous Structures for Tissue Engineering Scaffolds , WEN-TAU JUAN, KUO-YUAN CHUNG, Institute of Physics, Academia Sinica, Taipei, Taiwan, NARAYAN MISHRA, Dept. of Paper Technology, Indian Institute of Technology, Roorkee, KENG-HUI LIN, Institute of Physics, Academia Sinica, Taipei, Taiwan — A simple, inexpensive and fast microfluidic method to fabricate three-dimensional ordered macroporous gel is demonstrated using alginate as the scaffold material. The microfluidic device consists of two concentric micropipettes where one is nested inside the other. Nitrogen gas and aqueous alginate solution with Pluronic F127 are pumped through the inner and the outer channel respectively. Under appropriate conditions, bubbles of a uniform size are generated within the device at few thousand Hz. We show the control over bubble size by the gas pressure and quantitatively predict the size dependence from the geometry of fluidic device. Monodisperse bubbles are collected and self-assemble into crystal structures as wet foam. The alginate solution between bubbles is crosslinked by divalent calcium ions and turns into 3D ordered macroporous gel where the pores are highly interconnected. The pore size can be directly controlled by the bubble size which ranges from few tens microns to few millimeters. This technique promises a versatile and robust way to make 3D ordered tissue engineering scaffolds.

11:51AM B8.00004 Five-fold attractor in two-dimensional diffusion processes.[1] , GUILLERMO RAMIREZ-SANTIAGO, Instituto de Fisica, UNAM, CARLOS I. MENDOZA, Instituto de Investigaciones en Materiales, UNAM — We introduce an algorithm to generate two-dimensional diffusion-limited star-branched polymers (DLSP) attaching monomers successively to a central colloidal particle with any desired number of reactive sites. The proposed algorithm produces star-shaped aggregates whose final structure at relatively large distances from the central colloid has five-fold symmetry independently of the initial number of reactive sites. Therefore, the final morphology can be considered as a universal attracting distribution for this irreversible diffusion-limited aggregation process.

[1]We acknowledge partial financial suport by DGAPA-UNAM proyect IN-107607 and CONACYT 43596-F.

12:03PM B8.00005 Template-Guided Langmuir-Blodgett Deposition of Colloidal Particles , JAEHYUN HUR, YOU-YEON WON, Purdue University — We present a new method of fabricating highly-ordered two-dimensional (2D) colloid crystals with non-closed-packed symmetries. In this method, using the Langmuir-Blodgett (LB) monolayer deposition technique, we transfer a Langmuir monolayer of colloidal particles constructed at the air-water interface onto a substrate which contains micro-fabricated topological patterns. We demonstrate that by using this template-guided LB deposition method, a perfect single 2D colloid crystal structure that is homogeneous throughout the entire area of the patterned substrate can be economically fabricated under appropriate LB processing conditions. We investigate the effects of various control parameters (such as the initial particle density at the air-water interface, the substrate lifting speed, and the humidity condition during the LB monolayer deposition) on the structural properties of the resultant LB colloid monolayer. As the compression area or the lifting speed is increased, the average density of the deposited particles in the resultant LB colloid monolayer becomes reduced. The evaporation of water causes an undulation in the deposited particle density profile along the substrate lifting direction. We present a theoretical model which can quantitatively explain all these experimental observations.

12:15PM B8.00006 Clustering in Hard Core/Soft Shoulder Lattice Gas Models , PAUL D. BEALE, University of Colorado at Boulder, CHARLES A. SIEVERS, MATTHEW A. GLASER — Isotropic hard core/soft shoulder interacting particle models have been shown to display a wide variety of thermodynamic phases: structured liquids, micellar solids, layered and columnar liquid crystals, and a variety of modulated solid phases. We have explored the phase diagram of a class of lattice gas models that are designed to approximate continuum models. We use generalizations of Baxter's hard hexagon model on a two-dimensional hexagonal lattice to model the hard core repulsions. The longer-ranged repulsive soft shoulder is included to induce a Klein/Likos clustering instability. The clustering instability creates softly interacting fluidic micelles, as well as several type of modulated solid phases. The lattice gas model allows for efficient Monte Carlo simulation in order to quickly explore the phase diagram. Two dimensional lattice gas models typically only display liquid phases with short-range order and solids with long-range order that is commensurate with the underlying lattice. Preliminary results indicate the model exhibits soft solid phases composed of fluidic micelles that form a quasi-long ranged solid phase characteristic of continuum solid phases in two dimensions. We will also present a mean field theory analysis of the initial clustering instability.

12:27PM B8.00007 Elastic Theory of Defects in Toroidal Crystals , LUCA GIOMI, MARK BOWICK, Syracuse University — Crystalline assemblages of identical sub-units packed together and elastically bent in the form of a torus have been found in the past ten years in a variety of systems of surprisingly different nature, such as viral capsids, self-assembled monolayers and carbon nanomaterials. We investigate the structural properties of toroidal crystals and we provide a unified description based on the elastic theory of defects in curved geometries.

12:39PM B8.00008 Two-dimensional hopping of aqueous colloidal clusters on commensurate surface wells. , MINSU KIM, Physics, UIUC, STEPHEN ANTHONY, Chemistry, UIUC, STEVE GRANICK, Material Science and Engineering, UIUC — Hopping of colloidal clusters in various shapes and sizes that are mainly confined within commensurate surface wells except for diffusing between them by Brownian motion is studied. The mobility of clusters decreases nonmonotonically with increasing cluster size. The mobility proceeds, depending on cluster shape, by different jumping mechanisms such as zigzagging or translation without rotation; this produces nonmonotonic changes of mobility when, at fixed cluster size, cluster shape varies. Unlike atomic clusters that change configuration and dissociate easily, these colloidal clusters are very stable and each type of jump can be identified separately. Hopping rate, diffusion and different jumping mechanisms that are associated with them will be discussed for various sizes and shapes of clusters.

12:51PM B8.00009 Complexity from Specificity: Light Scattering and Colloidal Studies of Dscam Self-Association , JESSE COLLINS, Harvard School of Engineering and Applied Science (SEAS), NATALIE ARKUS, Harvard SEAS, GUANGNAN MENG, Harvard Physics, MICHAEL BRENNER, Harvard SEAS, DIETMAR SCHMUCKER, Dana Farber Cancer Institute, VINOTHAN MANOHARAN, Harvard SEAS and Department of Physics — The self-assembly of complex structures from nanometer-sized building blocks is of great technological importance(i.e. for the development of tissue scaffolds and photonic crystals) and is of significant basic scientific interest. Here I present light scattering and colloidal aggregation studies of Dscam, a protein with over 18,000 splice variants which all (or almost all) exhibit exclusively homophilic binding, and which is necessary for the generation of structural complexity in the brain of insects. Static and dynamic light scattering data reveal the statistical mechanical properties of Dscam self-association, including the free energy, second virial coefficient, and oligomer molecular weight. Finally, I demonstrate how to exploit Dscam's unprecedented level of molecular diversity and specificity for the self-assembly of custom nano- and micro-structures out of Dscam-conjugated colloids.

1:03PM B8.00010 Non-spherical Depletants in Colloidal Suspensions[1] , STEPHEN BARR, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — We investigate the effective interactions between spherical colloids induced by rigid rod-like depletants. The size disparity between the colloids and the rods makes conventional simulation methods inefficient. We overcome this by extending the generalized geometric cluster algorithm for colloidal suspensions [J. Liu and E. Luijten, Phys. Rev. Lett. **92**, 035504 (2004)] to systems of non-spherical particles. We investigate both uncharged and charged colloids and rods, where the electrostatic potential is modeled through a screened interaction. The dependence of the induced depletion potential on both the strength and the range of the electrostatic interactions is quantified. In case of a rod-sphere repulsion, the depletion attraction between the colloids is enhanced as the screening length becomes larger, owing to the increased effective size of the rods. Systems with a rod-sphere attractions are also explored.

[1]This work is supported by the National Science Foundation through Grant No. DMR-0346914.

1:15PM B8.00011 Magnetically assembled "ring-shaped" colloidal particle structures , HUI SON, RANDALL ERB, Duke University, Mechanical Engineering and Material Science, BAPPADITYA SAMANTA, VINCENT ROTELLO, University of Massachusetts, Amherst, Chemistry, BENJAMIN YELLEN, Duke University, Mechanical Engineering and Material Science — We demonstrate a convenient method for assembling ring-shaped colloidal structures by applying uniform magnetic field to a mixture of 2.7-μm paramagnetic beads, 1-μm non-magnetic polystyrene beads, and a fluid dispersion of 10-nm iron oxide nanoparticles (i.e., ferrofluid). The ferrofluid serves as a magnetic contrast medium and induces dipole moments in both the paramagnetic and non-magnetic beads when an external magnetic field is applied. We discovered that for certain volume fractions of ferrofluid, the attractive forces generated between the smaller non-magnetic beads and the larger magnetic beads induce the non-magnetic particles to form a ring structure around the circumference of the paramagnetic beads. This method differs from similar self-assembly techniques in that the ring structures form solely through magnetic force, rather than depending on random motion and patterned bonding.

1:27PM B8.00012 Effects of surface biotin density on lipid monolayer-assisted 2D crystallization of streptavidin at the aqueous solution-vapor interface , MASAFUMI FUKUTO, MATTHEW LOHR, SUNTAO WANG, SUMIT KEWALRAMANI, LIN YANG, Brookhaven National Laboratory — Adsorption and two-dimensional (2D) crystallization of soluble protein streptavidin on a biotinylated lipid monolayer at an aqueous solution-vapor interface have been studied extensively since the 1990s. These previous studies, largely based on fluorescence microscopy and *ex-situ* electron microscopy measurements, revealed the effects of protein modifications and aqueous buffer conditions, such as pH and ionic strength. We have examined the dependence of 2D streptavidin crystallization on the areal biotin density in the lipid monolayer template, using Brewster-angle microscopy (BAM) and *in-situ* x-ray reflectivity and grazing-incidence x-ray diffraction (GID). The lipid monolayer consisted of a binary mixture of DMPC and DPPE-x-biotin, and the biotin density was controlled by varying the lipid composition while keeping the area per lipid fixed. Both BAM and GID results demonstrate that in order for 2D crystallization of streptavidin to occur, the surface biotin density must exceed a threshold, corresponding to approximately two biotins per protein. The results highlight the importance of well-defined molecular orientations to the 2D crystallization of proteins.

1:39PM B8.00013 Self-Assembly of 2D TMV Arrays on Substrate-Supported and Langmuir Lipid Monolayers , SUNTAO WANG, ANTONIO CHECCO, Brookhaven National Laboratory, ZHONGWEI NIU, QIAN WANG, University of South Carolina, MASAFUMI FUKUTO, LIN YANG, Brookhaven National Laboratory — Bionanoparticles (large proteins, viruses) are ideal building blocks for creating ordered two-dimensional (2D) arrays. These 2D protein crystals or ordered arrays are of great scientific and technological interest. Here, we demonstrate the use of in-situ x-ray scattering and Brewster angle microscopy (BAM) to monitor the formation of self-assembled, 2D ordered arrays by tobacco mosaic viruses (TMVs) on a lipid layer that was either supported by a solid substrate or formed at the liquid-vapor interface. The lipid monolayer not only confined the viral particles within a plane, but also provided the lateral mobility that is crucial for developing structural order. In-situ X-ray scattering was used to provide real time information on the structure of the virus array and guide optimizations of the surrounding chemical environment to improve in-plane structural order. The presence of Ca^{2+} ions is also essential to the formation of well ordered, closely packed 2D arrays of TMV. Atomic Force Microscopy was also used to directly image the final structure to provide real space confirmation of developed structural order.

1:51PM B8.00014 Non-equilibrium dynamics of virus capsid assembly , ARTEM LEVANDOVSKY, University of California Riverside — The process of self-assembly of nano-structures under non-equilibrium conditions has recently received a lot of attention in various fields. A viral shell (capsid) is, for sure, one of the most interesting biological structures that can spontaneously form (from statistical mechanics point of view) at the right pH and ionic strength. While the viral capsids are by far less complex than most other biological objects, the process of virus assembly remains poorly understood. Viruses are found to adopt many different shapes. The mechanisms involved in the self-assembly of capsids into a particular shape as well as the transitions from spherical to non-spherical shells are the subject of this presentation. We show that the kinetic formation of the protein building blocks into the intermediate states (dimmers, trimmers, pentamers and hexamers) can lead to the construction of shells with different morphologies.

2:03PM B8.00015 Thermal transport in colloidal silica system: effect of particle size and aggregation , GANG CHEN, FAN JIANG, Department of Physics and Astronomy, Ohio University, WENHUA YU, JULES ROUTBORT, Energy Systems Division, Argonne National Laboratory, DEPARTMENT OF PHYSICS AND ASTRONOMY, OHIO UNIVERSITY TEAM, ENERGY SYSTEMS DIVISION, ARGONNE NATIONAL LABORATORY COLLABORATION — Knowledge of the size and distribution of nanoparticles in solution is critical to understanding the observed enhancements of thermal conductivity in colloidal systems. We have applied small-angle x-ray scattering (SAXS) to study particle size and distribution of monodispersed and aggregated silica colloids. A hot-wire method has been used to measure thermal conductivity of the colloidal system. The results indicate that the thermal conductivity depends not only on the particle concentration, but also on the particle size and distribution. The experimental data contradict thermal transport models based on fluid interfacial layers or Brownian motion but shed light on the detrimental role of liquid-particle interface on the thermal transport properties.

Monday, March 10, 2008 11:15AM - 2:15PM –

Session B39 GSNP DFD: Focus Session: Collective Dynamics of Self-Driven Particles Morial Convention Center 231

11:15AM B39.00001 Polar and apolar active matter[1] , M. CRISTINA MARCHETTI, Syracuse University — Assemblies of interacting self-driven units form a new type of *active* soft matter with collective behavior qualitatively different from that of its individual constituents, nonequilibrium phase transitions, and unusual mechanical and rheological properties. Examples include cytoskeletal filaments crosslinked by motor proteins, bacterial colonies, migrating cells, and vibrated layers of granular rods. In this talk I will review our work on using nonequilibrium statistical physics to derive a continuum description of these systems from specific models of single particle dynamics. This approach aims at understanding the interplay between physical mechanisms (such as formation or loss of physical connections, excluded volume effects, directional forces) and biochemical or other processes in regulating the large-scale organization and function of active matter. I will contrast the behavior of units with a head and a tail that can exhibit a macroscopic polar state, where all organisms move coherently in a preferred direction, with that of units with head-tail symmetry, that can order in a nematic state, with no net motion on macroscopic scale. Finally, I will use a simple model of active rods on a substrate to discuss the interplay between equilibrium steric effects and self-propulsion in controlling order and fluctuations in active fluids.

[1]Work done with T. B. Liverpool, A. Ahmadi and A. Baskaran. Supported by DMR-0705105

11:51AM B39.00002 Swarming and swirling in self-propelled polar granular rods , ARSHAD KUDROLLI, Department of Physics, Clark University, Worcester, MA, GEOFFROY LUMAY, GRASP, Physics Department, University of Liège, B-4000 Liège,, DMITRI VOLFSON, LEV TSIMRING, Institute for Nonlinear Science, University of California, San Diego, La Jolla, CA 92093 — We discuss the dynamics of "self-propelled" polar rods experimentally and numerically. In the experiment, the polar motion was achieved by vibrating rods with asymmetric mass distribution. In the numerics, we postulate a driving force acting along the axis of the rod. We observe aggregation of rods at the boundaries because of the inability of rods to turn around and escape for high enough density under low noise conditions. As vibration strength and thus noise is increased, the aggregation reduces and a uniformly distributed state displaying local orientation order and swirls are observed. We observe greater than $\sqrt{n}$ density fluctuations which are in a qualitative agreement with the Toner-Tu model, but this agreement should not be over-emphasized since the model is directly applicable to a nematic regime. Our findings elucidate an important and interesting interplay between the shape and the directed motion in *realistic* self-propelled rods which affects the phenomenology of their collective dynamics.

12:03PM B39.00003 Rectification of Swimming Bacteria and Self Driven Particle Systems by Arrays of Asymmetric Barriers , CHARLES REICHHARDT, Los Alamos National Laboratory, Los Alamos NM, MEW BING WAN, Department of Physics, Washington University, St Louis, MO 63160, CYNTHIA OLSON REICHHARDT, Los Alamos National Laboratory, Los Alamos NM 87545, ZOHAR NUSSINOV, Department of Physics, Washington University, St Louis, MO, 63160 — We show that the recent experimental observation of the rectification of swimming bacteria in a system with an array of asymmetric barriers occurs due to the ballistic component of the bacteria trajectories introduced by the bacterial "motor." Each bacteria selects a random direction for motion and then moves in this direction for a fixed period of time before randomly changing its orientation and moving in a new direction. In the limit where the bacteria undergo only Brownian motion, rectification by the barriers does not occur. We also examine the effects of steric interactions between the bacteria and observe a clogging effect upon increasing the bacteria density.

12:15PM B39.00004 Delay induced instabilities in self-propelling swarming particles[1] , ERIC FORGOSTON, IRA SCHWARTZ, Naval Research Laboratory — We consider a general model of self-propelling biological or artificial individuals interacting through a pairwise attractive force in a two-dimensional system in the presence of noise and communication time delay. Previous work has shown that a large enough noise intensity will cause a translating swarm of individuals to transition to a rotating swarm with a stationary center of mass. In this work, we use numerical simulations to show that with the addition of a time delay, the model possesses a transition that depends on the size of the coupling parameter. This transition is independent of the swarm state (traveling or rotating) and is characterized by the alignment of all of the individuals along with a swarm oscillation. By considering the mean field equations without noise, we show that the time delay induced transition is associated with a Hopf bifurcation. The analytical result yields good agreement with numerical computations of the value of the coupling parameter at the Hopf point.

[1]Research supported by the Office of Naval Research and Army Research Office

12:27PM B39.00005 ABSTRACT WITHDRAWN –

12:39PM B39.00006 From Cannibalism to Active Motion of Groups , PAWEL ROMANCZUK, LUTZ SCHIMANSKY-GEIER, Institute of Physics, Humboldt University Berlin — The detailed mechanisms leading to collective dynamics in groups of animals and insect are still poorly understood. A recent study by Simpson et. al. suggests cannibalism as a driving mechanism for coordinated migration of mormon crickets [1]. Based on this result we propose a simple generic model of brownian particles interacting by asymmetric, non-conservative collisions accounting for cannibalistic behavior and the corresponding avoidance strategy. We discuss our model in one and two dimensions and show that a certain type of collisions drives the system out of equilibrium and leads to coordinated active motion of groups.
[1] Stephen J. Simpson, Gregory A. Sword, Patrick D. Lorch and Iain D. Couzin: *Cannibal crickets on a forced march for protein and salt*, PNAS, 103:4152-4156, 2006

12:51PM B39.00007 Spatial instability and bioturbulence in highly concentrated bacterial suspensions[1] , ANDREY SOKOLOV, IGOR ARANSON, Argonne National Laboratory — We present an experimental study of spatio-temporal organization and transition to complex collective swimming regimes in highly concentrated suspensions of Bacillus subtilis. Experiments are performed in a free-standing thin-film sample with controlled thickness. Novel non-invasive high-resolution optical coherence tomography technique is used to probe the density distributions in the film in real time. Increasing the film thickness beyond certain threshold triggered a transition from quasi-to-dimensional collective swimming to three-dimensional turbulent state which is attributed to Oxygentaxis. We have studied effect of the controlled oxygen concentration on the bacterial collective behavior and transition to turbulent bioconvection.

[1]This work was supported by U.S. DOE grant DE-AC02-06CH11357

1:03PM B39.00008 Non-Coalescent, Self-Assembling Water Drops: Phase transitions, flows and hydrodynamics , MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, School of Chemistry and Biochemistry, VIVEK SHARMA, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology, Atlanta GA 30332 — We study the collective nucleation, growth and self-assembly of non-coalescent water drops. These form and organize over evaporating polymer solutions exposed to a draft of moist air. The creation and evolution of a population of drops towards a closed packed array occurs in response to heat and mass fluxes involved in droplet condensation and solvent evaporation. We elucidate the kinetics and dynamics of droplet growth and assembly, by accounting for various transport and thermodynamic processes. These water drops template hexagonally ordered arrays of holes in polymer films. We thus have a useful and economical method for manufacturing porous films requiring only a drop of polymer solution (dilute) and a whiff of breath!

1:15PM B39.00009 Active nematics: fluctuations and coarsening[1] , SRIRAM RAMASWAMY, CCMT, Department of Physics, Indian Institute of Science, Bangalore 560 012, SHRADHA MISHRA, CCMT, Department of Physics, Indian Institute of Science, Bangalore 560 012, INDIA, FRANCESCO GINELLI, HUGUES CHATE, Service de Physique de l'Etat Condense', CEA/Saclay, 91191 Gif-Sur-Yvette, FRANCE, SANJAY PURI, School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110 067, INDIA — Nonequilibrium steady states with spontaneous nematic order are known to arise in collections of amoeboid cells as well as granular-rod monolayers. Recent studies [EPL 62 (2003) 196-202; PRL 96, 180602 (2006); PRL 97 (2006) 090602; Science 317 (2007) 105] have established that these states differ radically from thermal equilibrium systems of the same spatial symmetry. This talk will present results from our studies of microscopic as well as coarse-grained models of active nematics, highlighting the unique, fluctuation-dominated character of coarsening in these systems.

[1]Supported by CSIR and DST, India

1:27PM B39.00010 Long-range correlations in simulations of suspensions of swimming microorganisms , PATRICK UNDERHILL, University of Wisconsin-Madison, JUAN HERNANDEZ-ORTIZ, Universidad Nacional de Colombia Sede Medellin, MICHAEL GRAHAM, University of Wisconsin-Madison — Simulations of large populations of hydrodynamically interacting swimming particles have been performed at low Reynolds number in periodic and confined geometries. Our simulations show that the interactions of the particles lead to long-range spatial correlations in the fluid at scales larger than the size of a single organism. These long-range correlations lead to a large enhancement in the fluid transport properties. The diffusivity of passive, non-Brownian tracer particles diverges in the periodic geometry with increasing the simulation box size. This collective motion depends on the method the organism uses for propulsion. Simple scaling arguments have also been developed that can capture much of the physics of both the swimmer and tracer motions.

1:39PM B39.00011 Simulated Flocking Dynamics of 2D Self-propelled Hard Particles , DONALD BLAIR, University of Massachusetts Amherst — Following a recent demonstration of long-lived giant number fluctuations in a swarming, granular nematic (Narayan et. al, Science **317**, 105 (2007)), we perform 2D simulations of hard, self-propelled particles which communicate only through contact. We vary particle end-shape, polarity, and aspect ratio and explore the effects on order, on the development of density fluctuations, and on the evolution of the swarm boundary. Connections to various forms of active matter (swimming bacteria, crawling cells) will be discussed.

1:51PM B39.00012 Cell swarming leads to vortex flow in early embryo formation , ARIEL BALTER, Biocomplexity Insittute, Indiana University, JAMES A. GLAZIER, Biocomplexity Institute, Indiana University — A forming embryo can be though of as a confined region of incompressible medium. Vortex flow is observed in early embryo formation from *drosophila* fruit flies to mammals. The Navier-Stokes equation for fluid flow in a cavity is known to have stable vortex solutions. A model for cell motion in which cells move independently of their neighbors corresponds to high Reynolds number (*Re*) incompressible flow. An alternative cell-swarming model in which cells do influence their neighbors motion (through a mechanism known as *contact following*) corresponds to a flow model that is similar to low *Re* incompressible flow. Both models can potentially lead to stable vortex formation in a confined cavity. We investigate the applicability of both models to real biological systems

2:03PM B39.00013 Active elastic dimers: self-propulsion and current reversal on a featureless track , VIJAY KUMAR KRISHNA MURTHY, SRIRAM RAMASWAMY[1], CCMT, Dept. of Physics, Indian Institute of Science, Bangalore 560012., MADAN RAO[2], Raman Research Institute, Bangalore 560080. — Directed motion without an imposed external gradient is seen not only in living systems but also in agitated granular matter. The essential ingredients are an external energy input and an inherent asymmetry. Unlike traditional "Brownian ratchet models", the asymmetry of interest in the above systems is *internal* to the motile objects, and does not lie in an external periodic potential. In this work, we present a Brownian inchworm model of a self-propelled elastic dimer in the absence of an external potential. Nonequilibrium noise together with a stretch-dependent damping form the propulsion mechanism. Our model connects three key nonequilibrium features – position-velocity correlations, a nonzero mean internal force, and a drift velocity. Our analytical results, including striking current reversals, compare very well with numerical simulations. The model unifies the propulsion mechanisms of DNA helicases, polar rods on a vibrated surface, crawling keratocytes and Myosin VI. We suggest experimental realizations and tests of the model.

[1]Also at CMTU, JNCASR, Bangalore 560064.
[2]Also at NCBS (TIFR), Bangalore 560065.

Monday, March 10, 2008 2:30PM - 5:30PM –
Session D8 DFD GSNP: Focus Session: Granular Flows: Vibrated Morial Convention Center RO6

2:30PM D8.00001 Particle kinematics in a 3-dimensional vibration-fluidized granular medium[1] , HONG-QIANG WANG, NARAYANAN MENON, University of Massachusetts Amherst — We report a study by high speed video imaging of particle motions in the bulk of a three dimensional granular gas. We fluidise with intense vertical vibration, delrin spheres of diameter, d=1.6 mm confined in a 3-dimensional volume $(32d)^3$. We isolate particles moving in a thin slice of this volume by illuminating with a laser sheet. We have developed a new algorithm to track with sub-pixel precision particles that are only partially illuminated or eclipsed by other particles. We will present data in the low-volume fraction regime for spatial profiles of the the kinetic temperature and number density, as well as for the velocity distribution. These results will be compared to predictions from hydrodynamic models.

[1]This work was supported through NASA NNC05AA35A and NSF DMR 0606216.

2:42PM D8.00002 Heating mechanism affects equipartition in a binary granular system[1] , NARAYANAN MENON, HONGQIANG WANG, Dept of Physics, U. of Massachusetts — Two species of particles in a binary granular system typically do not have the same mean kinetic energy, in contrast to the equipartition of energy required in equilibrium. We investigate the role of the heating mechanism in determining the extent of this non-equipartition of kinetic energy. In most experiments, different species of particle are unequally heated at the boundaries. We show by event-driven simulations that this differential heating at the boundary influences the level of non-equipartition even in the bulk of the system. This conclusion is fortified by studying a numerical model and a solvable stochastic model without spatial degrees of freedom. In both cases, even in the limit where heating events are rare compared to collisions, the effect of the heating mechanism persists.

[1]We gratefully acknowledge support from NASA NNC05AA35A and NSF DMR 0606216

2:54PM D8.00003 Energy fluctuation, diffusivity and mobility in a 2D vibrated granular packing[1] , ERIC CLEMENT, RIM HARICH, ESPCI -Université Paris 6, NICOLAS VANDEWALLE, GEOFFROY LUMAY, GRASP-Université Liège — We present an experimental realization of a 2D vibrated granular packing. The new agitation method allows a spatially non synchronized influx of energy and the study of the vibrated packing at steady state. By image analysis of fast-camera movies, we obtain the velocity fluctuation spectra at different vertical levels and then, we separate the agitation velocities from the velocity fluctuations corresponding to the "thermalized" degrees of freedom. By measuring the corresponding particle diffusivities, we show that, in spite a large heterogeneity and anisotropy of the vibration, a relation between diffusivity and "thermalized" kinetic energy can be identified. We relate this type of fluctuation-dissipation relation to the mobility of macroscopic intruders of different sizes and weight moving in the vibrated granular packing.

[1]PMMH-ESPCI is the UMR 7636 of the CNRS.

3:06PM D8.00004 "Free Energy" in Vibrated Granular Non-Equilibrium Steady-States.[1] , MARK SHATTUCK, City College of New York — Equilibrium statistical mechanics is generally not applicable to systems with energy input and dissipation present, and identifying relevant tools for understanding these far-from- equilibrium systems poses a serious challenge. Excited granular materials or granular fluids have become a canonical system to explore such ideas since they are inherently dissipative due to inter-particle frictional contacts and inelastic collisions. Granular materials also have far reaching practical importance in a number of industries, but accumulated ad-hoc knowledge is often the only design tool. An important feature of granular fluids is that the driving and dissipation mechanisms can be made to balance such that a Non-Equilibrium Steady-State (NESS) is achieved. We present strong experimental evidence for a NESS first-order phase transition in a vibrated two-dimensional granular fluid. The phase transition between a gas and a crystal is characterized by a discontinuous change in both density and temperature and exhibits rate dependent hysteresis. We measure a "free energy"-like function for the system and compare and contrast this type of transition with an equilibrium first-order phase transition and a hysteretic backward bifurcation in a nonlinear pattern forming system.

[1]Supported by the National Science Foundation under Grant No. 0134837.

3:42PM D8.00005 Singular Energy Distributions in Granular Media , ELI BEN-NAIM, Los Alamos National Laboratory, ANNETTE ZIPPELIUS, Georg-August-Universitat — We study the kinetic theory of driven and undriven granular gases, taking into account both translational and rotational degrees of freedom. We obtain the high-energy tail of the stationary bivariate energy distribution, depending on the total energy E and the ratio $x = \sqrt{E_w/E}$ of rotational energy E_w to total energy. Extremely energetic particles have a unique and well-defined distribution $f(x)$ which has several remarkable features: x is not uniformly distributed as in molecular gases; $f(x)$ is not smooth but has multiple singularities. The latter behavior is sensitive to material properties such as the collision parameters, the moment of inertia and the collision rate. Interestingly, there are preferred ratios of rotational-to-total energy. In general, $f(x)$ is strongly correlated with energy and the deviations from a uniform distribution grow with energy. We also solve for the energy distribution of freely cooling Maxwell Molecules and find qualitatively similar behavior.

3:54PM D8.00006 Breathing Phenomena in Driven, Confined, Granular Chains[1] , ROBERT SIMION, Physics Dept, SUNY-Buffalo, ADAM SOKOLOW, Physics Dept, Duke University, SURAJIT SEN, Physics Dept, SUNY-Buffalo — We consider a tapered granular alignment where the spherical grains progressively shrink in radius by a factor q. The system has a hard wall at one end and a piston at the other. We assume that the piston can be used to impart a force F (time- dependent or otherwise) to an edge grain in the system. Extensive particle dynamics simulations and theoretical analysis reveal that such a system could revert back and forth between an oversqueezed state and a dilated state - i.e., "breathe." The breathing is strongly dependent on the driving. When driven with a constant force, we show that $TF^{1/6}$ is a constant for fixed q. More complex dynamics including nonlinear-resonance is observed when $F = F(t)$. The talk shall discuss the observed dynamical responses of the system.

[1]Research Supported by Army Research Office

4:06PM D8.00007 Numerical Study of Particle Damping Mechanism in Piston Vibration System via Particle Dynamics Simulation , XIAN-MING BAI, BINOY SHAH, LEON KEER, JANE WANG, RANDALL SNURR, Northwestern University — Mechanical damping systems with granular particles as the damping media have promising applications in extreme temperature conditions. In particle-based damping systems, the mechanical energy is dissipated through the inelastic collision and friction of particles. In the past, many experiments have been performed to investigate the particle damping problems. However, the detailed energy dissipation mechanism is still unclear due to the complex collision and flow behavior of dense particles. In this work, we use 3-D particle dynamics simulation to investigate the damping mechanism of an oscillating cylinder piston immerged in millimeter-size steel particles. The time evolution of the energy dissipation through the friction and inelastic collision is accurately monitored during the damping process. The contribution from the particle-particle interaction and particle-wall interaction is also separated for investigation. The effects of moisture, surface roughness, and density of particles are carefully investigated in the simulation. The comparison between the numerical simulation and experiment is also performed. The simulation results can help us understand the particle damping mechanism and design the new generation of particle damping devices.

4:18PM D8.00008 Breaking of granular jams with mechanical shocks , KE CHEN, ANDREW HARRIS, JOHN DRASKOVIC, PETER SCHIFFER, Department of Physics, Penn State University — We studied the brief granular flows initiated by breaking the jamming in a hopper using mechanical shocks. Jamming near the orifice of a hopper prevents granular materials from flowing spontaneously under gravity. Controlled mechanical shocks were applied from the bottom of the hopper to break the jamming and to initiate brief flows. The magnitude and the duration of the flows were measured. Preliminary results show that the probability of initiating a flow increases with the intensity of the shock, and reaches almost 100% at the highest shock intensities. We also investigated the flow probability as a function of the ratio between the diameters of the orifice and the bead. Statistical characteristics of the flow magnitude and duration evolve with shock intensity as well as the ratio between the diameters of the orifice and the bead. This research was supported by the NASA through grant NAG3-2384 and the NSF REU program through grant DMR 0305238.

4:30PM D8.00009 Spreading of a granular droplet , ERIC CLEMENT, PMMH, UMR7636 (CNRS), ESPCI Univ. P6-P7, 10 Rue Vauquelin, 75005 Paris, France, IVAN SANCHEZ, Centro de Fisica, IVIC, Apartado Postal 21827, Caracas 1020-A, Venezuela, FRANCK RAYNAUD, MSC, UMR 7057 (CNRS), Univ. Paris 7, JOSE LANUZA, BRUNO ANDREOTTI, PMMH, UMR7636 (CNRS), ESPCI Univ. P6-P7, 10 Rue Vauquelin, 75005 Paris, France, IGOR ARANSON, Materials Science Division, Argonne National Laboratory, Argonne, IL60439, USA — The influence of controlled vibrations on the granular rheology is investigated in a specifically designed experiment in which a granular film spreads under the action of horizontal vibrations. A nonlinear diffusion equation is derived theoretically that describes the evolution of the deposit shape. A self-similar parabolic shape (the"granular droplet") and a spreading dynamics are predicted that both agree quantitatively with the experimental results. The theoretical analysis is used to extract effective friction coefficients between the base and the granular layer under sustained and controlled vibrations. A shear thickening regime characteristic of dense granular flows is evidenced at low vibration energy, both for glass beads and natural sand. Conversely, shear thinning is observed at high agitation.

4:42PM D8.00010 2D granular avalanches with imposed vibrations , BRIAN UTTER, DAN AMON, James Madison University — We present work on a 2D free surface granular flow experiment under vertical vibration. The experiment consists of photoelastic grains in a 2D circular drum which is rotated at a constant rate (f $<$ 1 mHz). We measure time series of the slope, particle trajectories, and image the bulk force network. Avalanche and build-up distributions exhibit a power-law dependence as previously observed. We then vibrate the drum vertically to determine the effect of external vibrations on this "unjamming" transition. While larger vibrations destabilize the pile and decrease the maximum angle of repose, small vibrations lead to a strengthening of the pile and tend to increase the critical angle of failure. In the absence of vibration, when the drum is rotated opposite the direction of steady rotation, the critical angle of the first failure decreases slightly from the steady-state value due to the lack of an established steady-state force network.

4:54PM D8.00011 Bouncing trimer[1] , STEPHANE DORBOLO, FNRS, NICOLAS VANDEWALLE, University of Liege, GRASP TEAM — Trimers are composed of three stainless steel beads (1 cm of diameter) forming a solid equilateral triangle (2.5 cm of side). They are placed on a plate of an electromagnetic shaker. The system is shaken vertically. According to the acceleration, the trimer may spin, jump once every two periods or even every threee periods. Between these stable regimes, the system is chaotic. By measuring the time delay between two successive shocks (bead-plate), a mapping of the different regimes has been constructed. The spinning, 2-period and 3-period orbits occurs for the same acceleration whatever the frequency. However, the spin speed has been measured with respect of the frequency.

[1]SD thanks FNRS for financial support

5:06PM D8.00012 Dynamics of a single particle on a 2D driven granular lattice , JEFFREY OLAFSEN, KRISTIN COMBS, Department of Physics, Baylor University, G. WILLIAM BAXTER, Physics Department, Penn State Erie, The Behrend College — Previous measurements have demonstrated interesting behavior in a novel bi-layer granular gas experiment of mechanically shaken particles. The results are of importance because the two layers are in "thermal contact" and yet have very different dynamical behaviors. The lower layer of particles demonstrates velocity statistics that are strongly correlated and non-Gaussian, while the upper layer of particles concurrently demonstrates a lack of correlations and Gaussian velocity statistics. Details of the collisions within each layer (intralayer) and between the layers (interlayer) are clearly of interest to understand the simultaneous behavior. Measurements are made for a single particle in the upper layer to examine the effects of interlayer collisions. In addition, velocity statistics in both layers are analyzed to determine effects of the sidewalls.

5:18PM D8.00013 Structure and dynamics of a vibrated granular bead-chain , KEVIN SAFFORD, ARSHAD KUDROLLI, Clark Univ. Physics Dept., YACOV KANTOR, Tel Aviv Univ. Physics Dept., MEHRAN KARDAR, MIT Physics Dept. — We investigate the dynamics of a vibrated granular bead-chain with experiments and numerical simulations of random-walk models of polymers. Experiments are conducted with a chain composed of hollow 3 mm steel beads connected by flexible links confined to move on a 300 mm diameter rough circular bed. Observations made with digital imaging. We analyze the radius of gyration R_g, the structure factor of the chain configurations, and the diffusion of the center of mass. We find that R_g and the structure factor scale with the exponent $\nu \sim 3/4$, consistent with the two dimensional self-avoiding random-walk model. Further, we observe confinement effects in the scaling of R_g as the chain length increases relative to the size of the container. We perform simulations of non-self-avoiding walks confined to the same sized domain and find good agreement with experiment. The simulations show confinement effects dominate over self-avoided crossings in the experiments even when the length of chain is smaller than system size. We then experimentally examine the chain dynamics and find that the center of mass diffusion scales inversely as the length of the chain, consistent with the Rouse model of polymers. We observe an exponential decay in the the dynamical structure factor and compare this exponent with the measurement of the center of mass diffusion.

Monday, March 10, 2008 2:30PM - 5:30PM –
Session D9 DFD: Focus Session: Turbulence Morial Convention Center RO7

2:30PM D9.00001 Turbulent Viscosity Coefficient in 3-Dimesional Turbulence , HIROSHI SHIBATA, Sojo University — A new model for the large-eddy simulation (LES) is proposed. The LES has been accepted as the standard formalism for calculating observables concerning turbulence. In the application of the LES, several models are chosen. The purpose of the present paper is for us to propose one of the most physical models. The LES is usually written down as

$$\frac{\partial U_i}{\partial t} + (\vec{U}\cdot\vec{\nabla})U_i = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu_0 \Delta U_i - \frac{\partial Q_{ij}}{\partial x_j}. \quad (1)$$

The above equation is rewritten as

$$\frac{\partial U_i}{\partial t} + (\vec{U}\cdot\vec{\nabla})U_i = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu \Delta U_i \quad (2)$$

and ν is referred to as turbulent viscosity coefficient. The statistical mechanical method by Helfand[1] is extended replacing the relationship between the thermal velocity and the kinetic viscosity coefficient by the one between the turbulent velocity and the turbulent viscosity coefficient[2]. The major assumption here is the Gaussian statistics for the turbulent velocity. The concrete calculation using the lattice Boltzmann method is shown for 3-dimesional turbulence. [1] E. Helfand, Phys. Rev. 119,1(1960). [2] H. Shibata, J. Phys. Soc. Jpn. 76,024002(2007).

2:42PM D9.00002 Exploring the dynamics of the velocity gradient tensor , MARCO MARTINS AFONSO, CHARLES MENEVEAU, Dept. of Mech. Engineering - Johns Hopkins University - Baltimore, MD — The dynamics of the velocity gradient tensor is investigated by means of analytical and numerical computations. Our starting point is the Lagrangian evolution equation of this tensor and a model for the pressure Hessian and viscous term proposed in Chevillard and Meneveau (*Phys. Rev. Lett.* **97**, 174501, 2006). The model is based on the Recent Fluid Deformation (RFD) closure, which was introduced in order to overcome the unphysical finite-time blowup of the Restricted Euler model that neglects anisotropic pressure Hessian effects. Using matrix exponentials, the RFD closure takes into account both the geometry and the dynamics of the recent history of the deformation of a fluid particle, and requires the specification of a decorrelation time scale τ. When this time scale is chosen too short (or, equivalently, the Reynolds number is too high), unphysical statistics are observed in the model. In order to understand this model in greater detail, the original, full matrix-exponential-based model is compared with its power- series expansion for small τ. In particular, the time evolution in the so-called R-Q plane is studied for the two approaches, and also, the effects of adding a Gaussian white noise are examined.

2:54PM D9.00003 The Generalized Fractal Dimensions of a 2-D Compressible Turbulence[1] , JASON LARKIN, WALTER GOLDBURG, University of Pittsburgh, MAHESH BANDI, Los Alamos National Laboratory — Steady-state turbulence is generated in a tank of water 1m x 1 m x 0.3 m and the trajectories of particles floating on the surface are tracked in time. Initially the floaters are uniformly distributed. As time goes on they coagulate and form a fractal structure. The surface pattern reaches a steady state in approximately $t^* = 1$ s. In the time interval $0 \lesssim t \lesssim 2t^*$, measurements are made of the generalized fractal dimensions $D_q(t)$ of the floating particles starting with the uniform distribution $D_q(0)$ =2. In the steady state, the pattern formed by the floaters continues to fluctuate at a time scale dictated by the underlying turbulent flow. This time scale is also of the order of 1 s. To understand the origin of the coagulation phenomenon, one must remember that the floaters form a compressible system, unlike the water molecules that drive them. The time evolution of the $D_q(t)$ are measured for a range of q less than 10. The coagulated particles form into string-like structures having values of D_q ranging down to approximately 1.5.

[1]Funding from the National Science Foundation

3:06PM D9.00004 Particle Dynamics in Turbulence , HAITAO XU, Max Planck Institute for Dynamics and Self-Organization — The interaction between particles and turbulence features in many environmental and engineering problems, e.g., the formation of rain, the dispersion of particulate pollutants, and sedimentation in rivers and oceans. In addition, tracer particles are routinely used in scientific research to study the flow itself. Understanding the behavior of particles in turbulent flows is not only an important practical problem, but also an intriguing scientific challenge. Our group has developed a three-dimensional Lagrangian Particle Tracking (LPT) system. Using high speed CMOS cameras, the system is capable of following simultaneously hundreds of particles in a turbulent flow with Taylor microscale Reynolds number R_λ up to 10^3. The LPT measurements provide both single- and multi-particle statistics following Lagrangian trajectories, at temporal resolutions better than the Kolmogorov time scales of the turbulence. Using the LPT system, we investigated the Lagrangian properties of turbulence by tracking tracer particles seeded in the flow. In the study of turbulent relative dispersion, our measurement of the separation of pairs of fluid elements in turbulence demonstrated that only when the separation between a time scale related to the initial separation between the pair and the turbulence integral time scale is large enough, or equivalently, at very large Reynolds numbers, the long-believed Richardson's t^3 law may be observed. Furthermore, measurements of multiple particles in the flow showed the evolution of geometric structures in turbulence. Due to its ability to follow individual particles, the LPT system is an ideal tool to study the behavior of non-tracer particles in turbulence. The inertial particles have density different from the fluid, but size smaller than the Kolmogorov length scale of turbulence. On the other hand, neutrally buoyant particles with size larger than the Kolmogorov scale behave very differently from inertial particles. We will present results from both cases.

3:42PM D9.00005 Craig's XY-distribution and the statistics of Lagrangian power in two-dimensional turbulence.[1] , COLM CONNAUGHTON, University of Warwick, MAHESH BANDI, Los Alamos National Laboratory — We study the probabilility distribution function (PDF) of injected power in numerical simulations of stationary 2D turbulence in the Lagrangian frame. The simulation mimics an electromagnetically driven fluid layer, a well-documented system for generating 2D turbulence in the laboratory. The forcing and velocity fields in the numerics are close to Gaussian, but the injected power PDF is sharply peaked at zero (suggesting a singularity) with asymmetric exponential tails. Large positive fluctuations are more probable than large negative ones leading to a net positive mean energy input. The main features of the power distribution are well described by Craig's XY distribution for the PDF of the product of two correlated normal variables. We show that the power distribution should exhibit a logarithmic singularity at zero and decay exponentially for large absolute values of the power. We calculate the asymptotic behaviour and express the asymmetry of the tails in terms of the correlation coefficient of the force and velocity and compare the measured PDFs with theoretical calculations.

[1]This work was carried out under the auspices of the National Nuclear Security Administration of the U. S. Department of Energy at Los Alamos National Laboratory under Contract no. DE-AC52-06NA25396.

3:54PM D9.00006 Multiscale Sample Entropy of 2D Decaying Turbulence , ILDOO KIM, University of Pittsburgh, MATTHEW SHTRAHMAN, Western Pennsylvania Hospital, XIAO-LUN WU, University of Pittsburgh — Kolmogorov-Sinai entropy has been used to quantify degrees of complexity of spatiotemporally chaotic systems. However, it is not always convenient to implement in real experiments. Recently a Multiscale Sample Entropy (MSE) measure has been proposed, which allows easier analyses of time series. In this study, we have generated decaying turbulence in a two-dimensional soap film and have measured velocity fluctuations as functions of time and downstream distance using a laser Doppler velocimeter. We performed MSE analysis and found there is a time scale τ_0 at which the MSE is maximized. The value of τ_0, which correlates well with the large-eddy turn-over time, gets larger as turbulence decays. Other aspects of 2D turbulence are also analyzed using the velocity time series.

4:06PM D9.00007 Conformal invariance in two-dimensional turbulence , GUIDO BOFFETTA, University of Torino, Italy, DENIS BERNARD, Ecole Normale Superieure, Paris, ANTONIO CELANI, Institut Pasteur, Paris, GREGORY FALKOVICH, Weizmann Institute, Israel — We show that some features of two-dimensional turbulence display conformal invariance. In particular, the statistics of vorticity clusters in the inverse cascade is equivalent to that of critical percolation, one of the simplest universality classes of critical phenomena. Vorticity isolines are therefore described by Stochastic Loewner Equation curves SLE_6. This result is generalized to a class of 2d turbulent systems, including Surface Quasi-Geostrophic turbulence (which corresponds to SLE_4) and Charney-Hasegawa-Mima turbulence. The picture emerging from our results is that conformal invariance may be expected for inverse cascades in two-dimensions therefore opening new perspectives in our understanding of 2d turbulent flows. References:
D. Bernard, G. Boffetta, A. Celani, and G. Falkovich, Nature Physics **2** 124 (2006)
D. Bernard, G. Boffetta, A. Celani, and G. Falkovich, Phys. Rev. Lett. **98** 024501 (2007)

4:18PM D9.00008 Mixing and entrainment of oceanic overflows: Implications for global climate evolution , ROBERT ECKE, JUN CHEN, PHILIPPE ODIER[1], MICHAEL RIVERA, Los Alamos National Laboratory — Oceanic overflows are important elements of the Earth's global thermohaline circulation but the mixing and entrainment that occur for such overflows is poorly understood. In particular, as overflow water moves down an inclined slope its stability is governed by the competition between stratification, which stabilizes the flow, and vertical shear, which tends to destabilize the flow. The properties of our laboratory experiment are designed to mimic oceanic overflows to the extent achievable on laboratory-accessible length scales. The flow exits a nozzle and flows along an inclined plane such that there is gravitational forcing of the flowing gravity current. Velocity and density fields are measured simultaneous using particle image velocimetry and planar laser induced fluorescence. The flow structure and dynamics of mixing at different downstream locations are investigated for a different levels of stratification and shear. The role of turbulence is examined by comparing cases of turbulent and laminar gravity currents. The implication of these results for ocean simulations and for understanding global climate are discussed.

[1]permanent address: ENS Lyon, France

4:30PM D9.00009 Experimental Investigation of Homogeneity, Isotropy, and Circulation of the Velocity Field in Buoyancy-Driven Turbulence[1] , QUAN ZHOU, Department of Physics, the Chinese University of Hong Kong, CHAO SUN, Department of Applied Physics, University of Twente, KEQING XIA, Department of Physics, the Chinese University of Hong Kong — We present a direct multipoint velocity measurements of the 2D velocity field in the central region of turbulent Rayleigh- Bénard convection. The local homogeneity and isotropy of the velocity field are tested using a number of criteria and are found to hold to an excellent degree. The distribution of Γ_r is found to depend on the scale r, reflecting strong intermittency. Besides, the slight asymmetry of the distribution tails reflects the fact that the velocity circulation structure functions (CSFs) are able to capture anisotropic coherent structures, such as thermal plumes, more effectively than longitudinal structure functions (LSFs) and transversal structure functions (TSFs). It is further found that velocity circulation has the same anomalous scaling exponents as LSFs and TSFs for low-order moments ($p <= 5$). Whereas, for high-order moments ($p > 5$), the anomalous scaling exponents for circulation are found to be systematically smaller than those of LSFs and TSFs.

[1]This work was supported by the Hong Kong RGC (Grant Nos. CUHK 403705 and 403806).

4:42PM D9.00010 Flow mode transitions in turbulent thermal convection[1] , HENG-DONG XI, KE-QING XIA, The Chinese University of Hong Kong — We report an experimental study of structures and dynamics of the large-scale mean flow in Rayleigh-Bénard convection cells with aspect ratio (Γ) 1, 1/2 and 1/3. It is found that both a single circulating roll flow structure and two vertically stacked counter-rotating rolls exist in the three aspect ratio cells. The average percentage of time that the large-scale mean flow spends in the single-roll mode (SRM) and the double-roll mode (DRM) are 87.1% and 0.8% for $\Gamma = 1$, 69.5% and 7.9% for $\Gamma = 1/2$, and 26.7% and 34.1% for $\Gamma = 1/3$. Several routes of transitions among the different flow modes are identified. In addition, different structures for the DRM are found and their relative weights are determined. We also show direct evidence that the SRM is more efficient for heat transfer than the DRM. Although the difference is very small, it shows how changes in internal flow state can manifest in the global transport properties of the system. It is also found that the time interval between successive flow mode transitions has an exponential distribution, suggesting a Poisson process for the underlying dynamics. The duration of the flow mode transition is found to be log-normally distributed.

[1]This work was supported by the Research Grants Council of Hong Kong under Grant No. CUHK403705 and CUHK403806.

4:54PM D9.00011 The properties of elastic turbulence in semi-dilute polymer solutions , YONGGUN JUN, Physics of Complex Systems, Weizmann Institute of Science, VICTOR STEINBERG — We studied elastic turbulence in Karman swirling flow of semi-dilute polymer solution. The concentrations of polymer solution used in the experiment were 100, 300, 500, 700, and 900 ppm, and the velocity fields to calculate the rms of the gradients of the tangential velocity, ω_{rms}, were obtained using PIV. First we checked the saturation of ω_{rms} in the bulk, which represents the saturation of elastic stress. We found that $Wi_{bulk} = \omega_{rms}\tau$ saturates and approaches to unitary value as the polymer concentration increases. Here τ is the longest polymer relaxation time. Also we studied existence of the velocity boundary layer which is related to boundary layer of elastic stresses of elastic turbulence. The thickness of the boundary layer is the decreasing function of polymer concentration near the rotating upper plate but independent of concentrations near the wall.

5:06PM D9.00012 Geometry of plane Couette flow transitional turbulence , PREDRAG CVITANOVIC, JOHN GIBSON, JONATHAN HALCROW, Georgia Tech — We propose to use a hierarchy of exact unstable invariant solutions of the Navier-Stokes equations – corresponding to the recurrent coherent structures observed in experiments – to construct a description of the spatio-temporally chaotic dynamics of turbulent fluid flows as a walk through the space of such structures. This description should allow us to obtain quantitative predictions of transport properties of fluid flows such as bulk flow rate and mean wall drag.

5:18PM D9.00013 The heat transfer of water-based Al_2O_3 nanofluid in turbulent Rayleigh-Bénard convection[1] , SHENG-QI ZHOU, RUI NI, KE-QING XIA, Dept. of Physics, The Chinese University of Hong Kong, Hong Kong — We report experimental measurements of the convective heat transfer in water-based Al_2O_3 nanofluid in a cylindrical convection cell, which has 19 cm in both height and diameter. The nanofluid has been supplied by Nanophase Technologyies Inc. with an initial volume fraction (ϕ) 22%. It has been diluted into deionized water to obtain nanofluid of low volume fraction. The nominal diameter of Al_2O_3 particle is 45 nm. At the fixed heating power, $Q = 500W$, it has been found that the convective heat transfer coefficient ($h = Q/\Delta T$, ΔT is the temperature difference across the cell.) decreases to 2% when ϕ varies from 0.03% to 1.1%. At $\phi = 1.1\%$, we have measured the Nusselt number (Nu) as a function of Rayleigh number (Ra). It has been found that Nu of nanofluid collapses on the $Nu \sim Ra$ scaling curve of pure water at higher Ra (4×10^9 to 1×10^{10}). While the deterioration of convective heat transfer has been observed at lower Ra (8×10^8 to 4×10^9), and the deterioration becomes more pronounced with decreasing Ra. Additional measurement on the thermal and flow structures is in progress to understand the convective heat transport in nanofluid.

[1]Work supported by the CUHK direct grant 2060309 and United College grant CA11096.

Tuesday, March 11, 2008 8:00AM - 11:00AM –

Session H8 DFD: Focus Session: Glassy Dynamics in Colloids Morial Convention Center RO6

8:00AM H8.00001 Are colloidal and molecular glass formation related? , JOHAN MATTSSON, Chalmers University of Technology — Understanding why and how a glass is formed on a microscopic level remains an outstanding problem in condensed matter physics. A molecular glass is normally formed by cooling of a liquid. Upon entering the supercooled state, the structural dynamics slows down dramatically and eventually the liquid enters the non- equilibrium glassy state. On route towards the glass, the behaviour shows a range of highly general, near universal characteristics, such as stretched exponential behaviour of dynamic correlation functions and cooperative dynamics. Such generalities exist even though molecular glasses can be formed from liquids encompassing a wide range of molecular structures and interactions. Glass formation also occurs in altogether very different systems. One of the most interesting, both from a fundamental and an applications point of view, is that of colloidal suspensions. The high degree of control that can be achieved regarding colloidal particle size, shape and interactions makes this a fantastic model system in learning about glass-formation. We know that a range of properties observed during dynamic arrest in molecular systems for decreasing temperature are indeed mirrored in the arrest of a colloidal suspension upon increase of particle volume fraction. However, the richness in phenomenology observed for liquids has generally not been observed for colloids. We will discuss to what extent colloidal glass formation can be viewed as equivalent to molecular glass formation and present recent experimental work that suggests a remarkably direct connection.

8:36AM H8.00002 Applications of patchwork dynamics for glassy systems , CREIGHTON THOMAS, ALAN MIDDLETON, Syracuse University, OLIVIA WHITE, MIT — We present work on "patchwork dynamics" as a technique for studying the nonequilibrium properties of glassy systems. In patchwork dynamics, we replace local Monte Carlo simulations, which require exponentially long times to equilibrate at a given length scale, with exact equilibration on patches at a given length scale, which can be done rapidly in models such as the 2D Ising spin glass and disordered dimer models. We have demonstrated some interesting applications of patchwork dynamics to such systems: 1) as a heuristic ground state algorithm for the 2D Ising spin glass on a torus (for which there are no known fast exact algorithms) and the 3D Ising spin glass; 2) as a method to study aging effects, persistence, and memory in 2D and 3D Ising spin glasses; 3) as a sampling procedure to study the nonequilibrium properties of disordered dimer models at finite temperatures.

8:48AM H8.00003 Aging of a Binary Colloidal Glass , JENNIFER M. LYNCH, GIANGUIDO C. CIANCI, ERIC R. WEEKS, Department of Physics, Emory University — After having undergone a glass transition, a glass is in a non-equilibrium state, and its properties depend on the time elapsed since vitrification. We study this phenomenon, known as aging. In particular, we study a colloidal suspension consisting of micron-sized particles in a liquid — a good model system for studying the glass transition. In this system, the glass transition is approached by increasing the particle concentration, instead of decreasing the temperature. We observe samples composed of particles of two sizes ($d_1 = 1.0\mu m$ and $d_2 = 2.0\mu m$) using fast laser scanning confocal microscopy, which yields real-time, three-dimensional movies deep inside the colloidal glass. We then analyze the trajectories of several thousand particles as the glassy suspension ages. Specifically, we look at how the size, motion and structural organization of the particles relate to the overall aging of the glass. We find that areas richer in small particles are more mobile and therefore contribute more to the structural changes found in aging glasses.

9:00AM H8.00004 Structural signatures of dynamical heterogeneity in supercooled liquids , HEIDI PERRY, DAVID REICHMAN, Columbia University, Department of Chemistry — The underlying mechanism of the transition from liquid to glass is a long-standing open question in condensed matter physics. One long sought after clue to understanding the glass transition is a link between the structure and dynamics of a vitrifying fluid. The dynamics of a supercooled liquid near the glass transition have proven to be collective and heterogeneous, with the length scale of the dynamic regions increasing as the glass transition temperature is approached. Using computer simulations and a normal mode analysis, we demonstrate a link between the structural properties of a super cooled liquids and the collective dynamical regions.

9:12AM H8.00005 ABSTRACT WITHDRAWN –

9:24AM H8.00006 Fluctuations in the aging regime of a polymer glass[1] , AZITA PARSAEIAN, HORACIO E. CASTILLO, Department of Physics and Astronomy, Ohio University — We perform numerical simulations to investigate the fluctuations in the aging regime of a system of polymers which are interacting via the Lennard-Jones potential. We characterize how the fluctuations evolve by studying (i) probability distributions of local observables such as individual particle displacements Δx and intermediate scattering functions C_r associated with small regions and (ii) dynamic correlation functions such as the four-point density correlation $g_4(\mathbf{r}, t, t_w)$. We find that, similar to small molecule glasses, the probability distributions of local observables approximately collapse when the global two-time correlation $C_{\mathsf{global}}(t, t_w)$ is held fixed. We test for universality by comparing the probability distributions in the small molecule glass with those in the polymer glass.

[1]Work supported in part by DOE under grant DE-FG02-06ER46300 and by Ohio University.

9:36AM H8.00007 Equipartition theorem in glasses and liquids , VALENTIN A. LEVASHOV, TAKESHI EGAMI , University of Tennessee, RACHEL S. AGA , JAMES R. MORRIS, Oak Ridge National Laboratory — In glasses and liquids phonons have very short life-time, whereas the total potential energy is not linear with temperature, but follows the T**(3/5) law. Thus it may appear that atomic vibrations in liquids cannot be described by the harmonic oscillator model that follows the equipartition theorem for the kinetic energy and potential energy. We show that the description of the nearest neighbor oscillation in terms of the atomic level stresses indeed provide such a description. The model was tested for various pair-wise potentials, including the Lennard-Jones potential, the Johnson potentials, and only the repulsive part of the Johnson potential. In all cases each of the local elastic energies of the six independent components of the stress tensor is equal to kT/4, thus the total potential energy is equal to (3/2)kT. Thus this model provides the basis for discussing the thermodynamic properties of glasses and liquids based on atomistic excitations. An example of this model leading to the description of the glass transition temperature in metallic glasses is discussed [1].
[1] T. Egami, et al., Phys. Rev. B 76, 024203 (2007).

9:48AM H8.00008 Exceptionally Stable Organic Glasses with Low Enthalpy and High Kinetic Stability Prepared by Vapor Deposition , KENNETH L. KEARNS, STEPHEN F. SWALLEN, M.D. EDIGER, Department of Chemistry, University of Wisconsin-Madison, YE SUN, TIAN WU, LIAN YU, School of Pharmacy, University of Wisconsin-Madison — Vapor deposition can be used to prepare glasses of 1,3,5-(tris)naphthylbenzene (TNB) and indomethacin (IMC) that are much more stable than those created by cooling from the liquid. By controlling the temperature of the substrate and the deposition rate, the stability of the glass can be tuned. Glasses can be deposited with enthalpies as much as 10 J/g lower than the glass made by cooling the liquid. Vapor-deposited glasses can also be superheated well above the conventional T_g. The slow evolution from the low energy glass to the supercooled liquid is observed and can take tens of hours to evolve at temperatures near T_g+ 5 K. Trends in stability support an enhanced surface dynamics mechanism where we estimate the dynamics in the top 1 nm to be about 7 orders of magnitude faster than the bulk at T_g – 25 K. Vapor deposition has also allowed us to progress more than 40% towards the bottom of the amorphous potential energy landscape.

10:00AM H8.00009 Magnetic Analogies for the Dynamics of Glass Forming Liquids , JACOB STEVENSON, PETER WOLYNES, University of California San Diego — We present a direct mapping between the dynamics of glass forming liquids and a general random field / random coupling Ising model using the replica effective potential approach. Using the overlap between two structural states of a supercooled liquid we construct a constrained overlap free energy that can be mapped directly onto that of an Ising Hamiltonian. For a Lennard-Jones glass the fluctuations and mean values of the random fields and interactions place it within the universality group of the random field Ising magnet, not the Ising spin glass. This corresponds with the explanation for a random first order transition.

10:12AM H8.00010 Direct imaging of particle dynamics in attractive colloidal glasses[1] , PIOTR HABDAS, ANDRZEJ LATKA, Department of Physics, Saint Joseph's University, YILONG HAN, Physics Department, Hong Kong University of Science and Technology, AHMED ALSAYED, ARJUN G. YODH, Department of Physics and Astronomy, University of Pennsylvania — We use confocal and fluorescent microscopy to study the dynamics of glassy colloidal suspensions. The suspensions are composed of PMMA colloidal particles in density and index-of-refraction matched liquid and stained with a fluorescent rhodamine dye. A controllable depletion attraction is induced between hard-sphere PMMA particles by adding different amounts of polystyrene polymer to the suspension. Our dynamical measurements focus on jumps experienced by PMMA particles that escape the cage formed by its neighbors. We track these particles over time and correlate particle fluctuations with its changes in average position. We find that as the strength of the attractive potential increases, and the system enters an "attractive liquid" phase, the number of jumping particles increases. We calculate the distribution of particle jump sizes, time between jumps, and spatial distribution of particle jumps; these observations are compared to predictions of molecular dynamics simulations.

[1]This research was supported by an award from Research Corporation.

10:24AM H8.00011 Shear-induced ordering and vitrification of concentrated emulsions , JUNG-REN HUANG, THOMAS G. MASON, University of California-Los Angeles — Using time resolved light scattering, we investigate the degree of droplet deformation and ordering within concentrated oil-in-water emulsions subjected to oscillatory shear between parallel glass plates. We create uniform microscale droplets between the plates by rupturing a premixed emulsion of larger droplets at a fixed strain amplitude and frequency. Subsequently, by independently adjusting the strain amplitude and frequency and recording videos of the dynamic scattering pattern, we examine how the instantaneous applied shear and prior shear history influence the positional structure of the droplets. We also explore how the ordering of the emulsion droplets depends on the oil volume fraction, both above and below that associated with maximally random jamming of uniform hard spheres. The short-range stabilizing repulsion between oil droplets enforces ordering in the shear direction; yet, by contrast to sheared colloidal hard spheres, the deformability of the oil droplets allows concentrated emulsions to un-jam at sufficiently high shear rates. We propose a real-space model, based on the form factor of ellipsoidal droplets and structure factor of ordered, jammed, and un-jammed configurations, that is consistent with the observed light scattering patterns. This technique can be used to transform the structure of a uniform emulsion between ordered and disordered droplet configurations.

10:36AM H8.00012 Accentuated shear thinning of soft sphere suspensions , HANS M. WYSS, Harvard University, JOHAN MATTSSON, Chalmers University of Technology, Sweden, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology, GIOVANNI ROMEO, University of Naples Federico II, Italy, MELAKU MULUNEH, Harvard University, ZHIBING HU, University of North Texas, DAVID A. WEITZ, Harvard University — Suspensions of soft colloidal particles exhibit highly unusual rheological behaviors; surprisingly, despite the importance of these materials in a wide range of applications, the underlying physical mechanisms remain poorly understood. Experiments show that suspensions of soft particles exhibit a highly pronounced shear thinning; this decrease in viscosity with increasing shear rate far exceeds the shear thinning observed in suspensions of solid particles. We use soft microgel particles as a model system to elucidate this behavior. Our experimental system allows us to study the mechanical behavior both macroscopically and locally, at the scale of the colloidal particles themselves. We combine data obtained at different length scales to arrive at a simple picture of the observed accentuated shear thinning.

10:48AM H8.00013 Investigation of Rejuvenation and Overaging in Glassy Energy Landscapes , MYA WARREN, JOERG ROTTLER, University of British Columbia — Many glassy systems experience a change in their aging dynamics under the influence of mechanical load. It has long been known that large stresses can cause an apparent decrease in relaxation times (rejuvenation) in polymer glasses, but in colloidal glasses an increase (overaging) has also been observed depending on the strain amplitude. The conditions under which rejuvenation or overaging occur are not yet fully understood. Additionally, there is still considerable controversy over the nature of the resultant states. In order to gain intuition on these outstanding questions, we investigate the aging dynamics under load though stochastic simulations of the Soft Glassy Rheology (SGR) model. For both stress controlled and strain controlled loading, the SGR model exhibits clear regions of overaging and rejuvenation in a parameter space defined by the noise temperature, the quench history, and the strain. Additionally, results show that the states produced under loading are distinct from those that would naturally be visited during aging, and this has effects on the subsequent aging trajectory. Results from the energy landscape picture are compared to pertinent molecular dynamics studies.

Tuesday, March 11, 2008 8:00AM - 11:00AM –

Session H9 DFD: Instabilities and Fluid Dynamics Morial Convention Center RO7

8:00AM H9.00001 Low Frequency Oscillations in the Upper Atmosphere , SUDIP SEN, Kyoto University, Japan & Delhi University, India — No definitive theory exists which explains the origin of various low frequency oscillations observed in the ionosphere. Various authors, over the course of time, have put forward various explanations of this important phenomenon. Most recently it has been proposed that the spatial transverse shear in the parallel flow destabilizes many low frequency oscillations and this may be the origin of low frequency oscillations in the ionosphere [V V Gavrishchaka et al., Phys. Rev. Lett. **80**, 728 (1998) and Phys. Rev. Lett. **85**, 4285 (2000)]. In this article we review the various theories proposed till date to explain the origin of low frequency oscillations. We address the most recent theories in more detail. We show that the recent proposition of the spatial transverse shear might excite many instabilities may not be so obvious. Parallel flow curvature when taken into account might actually act to stabilize various instabilities [S. Sen et al. Phys. Rev. Lett. **88**, 185001 (2002)]. This article therefore concludes while much work has been done on the ionospheric oscillations much more work possibly remains to be done in this important area of space physics.

8:12AM H9.00002 Capillary-controlled instability in immiscible, parallel flow in porous media[1] , THOMAS RAMSTAD, ALEX HANSEN, Department of Physics, NTNU, N-7491 Trondheim and Numerical Rocks AS, Stiklestadveien 1, N-7041 Trondheim, Norway — When two immiscible fluids flow in parallel in a strongly wetted porous medium the global interface separating them tend to be kept in place by local capillary barriers. However, above a certain threshold in the flow rate, the separating interface may become unstable and mobilized. We study this instability theoretically by using a two-dimensional network as a model for porous media in a flow regime where capillary forces cannot be neglected. It is found that a boundary zone with a sharp saturation profile occurs between the regions originally saturated with either a wetting or a non-wetting phase. This zone has a well defined width and moves with constant speed towards the non-wetting region. In the opposite direction, a current of non-wetting bubbles is set up, but wetting bubbles into the non-wetting region are absent. This behavior is genuinely different from shear-induced Kelvin-Helmholtz instabilities.

[1]Supported by the Norwegian Research Council

8:24AM H9.00003 Stability of multi-layer Hele-Shaw flows with and without diffusion , PRABIR DARIPA, Texas A&M University — In this talk, we will provide some results in the context of multi-layer Hele-Shaw flows. We will address issues related to collective effects of individually unstable interfaces on the overall stability of multi-layer Hele-Shaw flows in the presence of interfacial surface tensions. We will also discuss complications in the analysis resulting from making, in the above set-up, individual layers also unstable. We obtain some sufficient conditions for suppressing instability of two-layer flows by introducing arbitrary number of constant viscosity fluid layers in between. For stabilization purposes, this condition allows selection of fluids in internal layers based on interfacial surface tensions and viscosities of fluids. Time permitting, we also examine the effects of species diffusion on the stability of the three-layer Hele-Shaw flows. This has relevance to enhanced oil recovery by polymer flooding. Analytically, we will prove the diffusive slow-down of unstable waves. It will be shown that a strong enough diffusion can almost stabilize the flow, though the magnitude of this diffusion coefficient required to completely stabilize the flow will depend on the magnitude of interfacial viscosity jumps and the viscosity gradient of the basic viscous profile of the internal layer. This work has been done in collaboration with Gelu Pasa.

8:36AM H9.00004 Meandering instability of a rivulet on a partially wetting incline , ADRIAN DAERR[1], MSC*, Denis-Diderot-University of Paris, LAURENT LIMAT[2], MSC*, CNRS & Denis-Diderot-University of Paris — It is common to observe small rivulets in sinks or on window-panes which follow sinuous paths (stationary or not) instead of flowing down along the direction of steepest slope. A laboratory experiment shows that these meandering rivulets exist only for certain ranges of the control parameters (flow rate and substrate inclination). The geometrical properties of the resulting paths can be understood in terms of force balances between inertia, capillarity and contact line pinning. The nature of the instability, i.e. why the straight rivulet becomes unstable, however remains unclear. We study the rivulet near the onset for meandering to understand the role of noise and surface defects.

[1]*CNRS UMR 7057
[2]*UMR CNRS 7057

8:48AM H9.00005 A quasi 2-D molecular dynamics study of the initiation and evolution of the Kelvin-Helmholtz instability , KYLE CASPERSEN, ROBERT RUDD, DAVID RICHARDS, JIM GLOSLI, Lawrence Livermore National Laboratory, JOHN GUNNELS, IBM, FREDRICK STREITZ, Lawrence Livermore National Laboratory — Typically hydrodynamic phenomena are modeled with continuum mechanics via integration of the Navier-Stokes (NS) equation or a closely related variant. However, as fluids are studied at smaller and smaller length scales atomistic effects can, and will, ultimately dominate; furthermore, even at micron scales it is not clear that the NS equation provides a complete description of the fluid, e.g. due to the initiation of instabilities at the molecular scale in initially quiescent fluids. To assess the effect of atomistic behavior on one particular hydrodynamic phenomenon–the Kelvin-Helmholtz instability–we have performed a very large molecular dynamics simulation of molten metals undergoing shear flow. Nine billion copper and aluminum atoms were sheared at a speed of 2000 m/sec for a total simulated time of more than a nanosecond. We present here results showing the initiation of the instabilities, the crossover to hydrodynamics, and the evolution and scaling behavior of the KH instability in a quasi 2-D geometry. Prepared by LLNL under Contract DE-AC52-07NA27344.

9:00AM H9.00006 A fully 3-D molecular dynamics study of the initiation of the Kelvin-Helmholtz instability[1] , ROBERT E. RUDD, K.J. CASPERSEN, D.F. RICHARDS, J.N. GLOSLI, Lawrence Livermore National Laboratory, J.A. GUNNELS, IBM, F.H. STREITZ, Lawrence Livermore National Laboratory — The modeling of hydrodynamic phenomena has almost exclusively been the purview of continuum mechanics, specifically, through the use of the Navier-Stokes equation and closely related variants. Nevertheless, at the smallest length scales, where atomistic effects become important, it is not clear that this continuum approach provides a complete description of fluid behavior. To understand the effects of atomistics, we have performed a 62.5-billion-atom, fully 3-D molecular dynamics simulation of a cubic micron of molten copper and aluminum. The shear flow at 2 km/s exhibits complex phenomena associated with a Kelvin-Helmholtz (KH) instability. In this presentation we will discuss the initiation and early evolution of the KH instability, focusing specifically on the effects of full atomistic resolution.

[1]This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.

9:12AM H9.00007 Bubble Pinch-off at High Pressures , J.C. BURTON, P. TABOREK, University of California, Irvine — Previously we have studied the pinch-off of conventional air bubbles in water [1]. For inviscid fluids, the shrinking of the neck radius of the bubble can be described by a power-law in time with an exponent close to 1/2. As the density of the interior gas is increased, instabilities are expected to occur in the liquid/gas interface [2]. We present high-speed videos and numerical simulations of the pinch-off of high-pressure gaseous bubbles in and exterior inviscid fluid. The density ratio between the exterior fluid and interior gas is D=ρ_{ext}/ρ_{int}. In the simple case of small D$\sim$0.001, the pinch-off is similar to that of a water drop pinching-off in air, while at large D$\sim$1000, the pinch-off is that of an air bubble in water. By using sulfur hexafluoride as a working gas, we are able to span a wide ranging of density ratios simply by increasing the pressure of the gas. A high-pressure ($\sim$30 atm) chamber with optical access through sapphire windows was constructed in order to view the pinch-off. The numerical simulations are performed assuming perfectly inviscid fluids using boundary-integral techniques. Instabilities in the interface are seen for intermediate density ratios. Comparisons between experimental and numerical results will be discussed.
[1] J.C. Burton, R. Waldrep, and P. Taborek. Phys. Rev. Lett. 94, 184502, (2005).
[2] D. Leppinen and J.R. Lister. Phys. Fluids 15, 568, (2003).

9:24AM H9.00008 First order phase transition in the height of a meniscus in a tapered capillary , MICHAEL PETTERSEN, Washington and Jefferson College, ETIENNE ROLLEY, Laboratoire de Physique Statistique, Ecole Normale Superieure — When a fluid rises in a capillary of non-uniform cross section, additional terms arise in the balance of capillary forces, compared to the case of a capillary of uniform cross section, due to the changing area of the meniscus. Recently, it has been pointed out that this can lead to a first order phase transition, resulting in a discontinuous jump in the equilibrium position of the meniscus. We present the results of an experiment using isopropanol and silicone oil in cones with apex upwards of different opening angles. The cone is slowly lowered into the liquid using a translation stage. We have measured the capillary rise in this geometry, and observed the predicted phase transition.

9:36AM H9.00009 Luminescence from Laser-Induced Bubbles in Water-Glycerol Mixtures: Effect of Viscosity[1] , ERIN ENGLERT, ALLISON MCCARN, GARY A. WILLIAMS, Dept. of Physics and Astronomy, UCLA — We have studied the luminescence emitted from collapsing laser-induced bubbles in water-glycerol mixtures, as a function of the mixture concentration and applied hydrostatic pressure. The primary effect of increasing the glycerol concentration is to increase the viscoslty of the fluid. We find that the pulse duration of the luminescence increases by more than a factor of two as the concentration increases up to 33% by volume, where the viscosity is nearly four time that of pure water. At higher concentrations the pulse duration remains nearly unchanged, until no luminescence can be observed at concentrations above 60% (viscosity greater than 15 times that of water). The pulse duration further increases with applied pressures up to 8 bars, similar to that seen earlier in pure water.

[1]Work supported by the NSF, DMR 05-48521, and one of us (A. M.) acknowledges support from the UCLA REU program.

9:48AM H9.00010 Hysteretic and Chaotic Dynamics of Viscous Drops in Creeping Flows with Rotation[1] , YUAN-NAN YOUNG, Depatment of Mathematical Sciences, New Jersey Institute of Technology, JERZY BLAWZDZIEWICZ, Department of Mechanical Engineering, Yale University, VITTORIO CRISTINI, University of Texas, Houston, ROY GOODMAN — It has been shown in our previous publication (Blawzdziewicz et al 2003) that high-viscosity drops in two dimensional linear creeping flows with a nonzero vorticity component may have two stable stationary states. One state corresponds to a nearly spherical, compact drop stabilized primarily by rotation, and the other to an elongated drop stabilized primarily by capillary forces. Here we explore consequences of the drop bistability for the dynamics of highly viscous drops. Using both boundary-integral simulations and small-deformation theory we show that a quasi-static change of the flow vorticity gives rise to a hysteretic response of the drop shape, with rapid changes between the compact and elongated solutions at critical values of the vorticity. In flows with sinusoidal temporal variation of the vorticity we find chaotic drop dynamics in response to the periodic forcing. A cascade of period-doubling bifurcations is found to be directly responsible for the transition to chaos. In random flows we obtain a bimodal drop- length distribution. Some analogies with the dynamics of macromolecules and vesicles are pointed out.

[1]This work is supported by NSF.

10:00AM H9.00011 A Temporal Period Doubling Route to Spatiotemporal Chaos in a System of Amplitude Equations for the Nematic Electroconvection[1] , IULIANA OPREA, GERHARD DANGELMAYR, Colorado State University — We analyze the transition from periodic solutions to spatiotemporal chaos in a system of four globally coupled Ginzburg Landau equations describing the dynamics of instabilities in the electroconvection of nematic liquid crystals, in the weakly nonlinear regime. If spatial variations are ignored, these equations reduce to the normal form for a Hopf bifurcation with O(2) x O(2) symmetry. Coexistence of low dimensional and extensive spatiotemporal chaotic patterns, as well as a temporal period doubling route to spatiotemporal chaos, corresponding to a period doubling cascade towards a chaotic attractor in the normal form, are also identified and discussed, for values of the parameters including experimentally measured values of the nematic I52.

[1]Research supported by NSF/DMS-407418.

10:12AM H9.00012 Angular momentum transport in complex fluids[1] , XIAOYU ZHENG, Kent State University, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU, MICHAEL SHELLEY, Courant Institute of Mathematical Sciences, NYU — When dyes are dissolved in nematic liquid crystals, the light intensity required for the optical Freedericksz transition can be dramatically decreased. This is due to the torque exerted by the dye on the liquid crystal. The dye molecules absorb light energy and rotate; torque balance is mediated by angular momentum transport from the cell walls via shear flow generated by the rotation [1]. We present a model which accounts for the transport of angular momentum caused by singular vortices present in these complex fluids. The singular vortices generate flow, and are transported by the flow which they generate. For simple fluids, the distribution of vorticity satisfies the biharmonic equation in the Stokes limit, which can be solved analytically. In the case of the non-Newtonian fluids, such as liquid crystals, Leslie-Ericksen continuum theory is used to describe the interactions between the rod-like molecules. [1] P. Palffy-Muhoray, T. Kosa and Weinan E, "Brownian Motors in the Photoalignment of Liquid Crystals", *Appl. Phys. A* **75**, 293-300 (2002).

[1]This work was supported by the NSF under grant DMR 0606357.

10:24AM H9.00013 Particle Dynamics in Bi-Disperse Liquid Fluidized Beds , PHIL SEGRE, Emory University Physics Dep, GARY L. HUNTER, JAMES DAVIDHEISER, ELIZABETH BAKER, Emory Univ. Physics Dep. — We study particle velocities and concentration profiles of mixtures of 2 different sized particles in concentrated liquid fluidized beds. For binary systems of particles of the same density, we find that there is always a complete phase separation in the bed. The larger particles occupy a zone in the lower part of the bed, and the smaller ones a zone in the upper part. For binary systems of particles of *different* density materials, conditions are found where the binary particles are either fully separated, partially mixed together, and at a single point called the inversion point, fully mixed into a one phase state. Results will be presented on the phase diagrams of several binary suspensions as well as the properties of the velocity fluctuation magnitudes and spatial correlation lengths.

10:36AM H9.00014 Polygonal hydraulic jump on microtextured surfaces , EMILIE DRESSAIRE, LAURENT COURBIN, SEAS, Harvard University, JEROME CREST, Dept. of Mechanical Engineering, MIT, HOWARD A. STONE, SEAS, Harvard University — Fluid motion can be drastically influenced by the nature of boundaries. For instance, we have shown recently [1] that a substrate with a regular array of micron-size posts can cause partially wetting fluids to take on polygonal shapes. Here, we report on the hydraulic jump that occurs when a water jet impinges a topographically patterned surface, i.e. an array of micron-size posts arranged on square or hexagonal lattice. By varying the topographic features (shape and height of the posts, lattice distance) and the jet properties (size of the nozzle, flow rate), we obtain a variety of stable shapes including hexagons, eight corner stars and circles. We rationalize our results by taking into account a fluid velocity that depends on the orientation of the lattice.

[1]L. Courbin, E. Denieul, E. Dressaire, M. Roper, A. Ajdari and H.A. Stone, Nature Mater. **6**, 661 (2007)

10:48AM H9.00015 Enstrophy-constrained stability analysis of beta-plane Kolmogorov flow with drag , YUE-KIN TSANG, WILLIAM YOUNG, Scripps Institution of Oceanography, UCSD — For forced two-dimensional flows, energy injected at a certain wavenumber is redistributed to both larger and smaller wavenumbers. This results in a constraint on the time evolution of the difference between the energy and enstrophy. By incorporating this constraint in an energy stability analysis of Kolmogorov flow on a beta-plane with drag, we establish an extended region in the parameter space of beta and the drag coefficient where the flow is stable to arbitrary perturbations. Complementary to this nonlinear stability result, linear instability theory is used to determine the part of the parameter space where the flow is unstable to infinitesimal perturbations. We also find that the most unstable mode in the linear stability analysis has a discontinuous change in structure as beta decreases below a certain value. Results from numerical simulations spanning the parameter space support the theoretical predictions.

Tuesday, March 11, 2008 8:00AM - 11:00AM –

Session H16 DBP DFD: Focus Session: Biochip Physics I Morial Convention Center 208

8:00AM H16.00001 Size Scaling of Protein Sensitivity on the BioCD[1] , KEVIN O'BRIEN, MING ZHAO, XUEFANG WANG, DAVID NOLTE, Purdue University — We investigate size scaling of the surface-height sensitivity of spinning-disk interferometry (SDI) implemented on the in-line-quadrature BioCD as a function of laser focal radius. The in-line-quadrature BioCD consists of a silicon wafer with a 120 nm layer of silicon dioxide that creates a quadrature condition between the incident and reflected light. When a laser beam is focused on the BioCD, proteins printed on the silicon dioxide substrate create a phase shift leading to quadrature interference, which is detectable in the far field as an intensity shift. The purpose of this scaling experiment is to determine the practical and fundamental limits on the sensitivity of the BioCD, and how those limits change as a function of the size of the focal spot. We imaged a single 100 micron wide protein spot with focal spot sizes of 1, 5 and 10 microns and observe a square-root scaling as a function of the number of pixels per protein spot.

[1]NSF REU Program

8:12AM H16.00002 Detection Limits of Captured Protein on the BioCD , DAVID NOLTE, XUEFANG WANG, KEVIN O'BRIEN, MING ZHAO, Purdue University — The BioCD is an interferometric biosensor that detects protein captured by antibody arrays. The sensor readout is performed on a spinning disc using a common-path interferometric configuration that is stable and sensitive to sub-monolayer coverage of captured protein. Protein is detected using phase quadrature that converts phase to intensity modulation using local generation of signal and reference to lock the relative phase of the waves. The purpose for spinning is to move far from 1/f noise to achieve high surface mass sensitivity. Several different classes of the BioCD have been developed, differentiated by the means of generating the phase-locked reference. These include the microdiffraction (MD) class, the phase contrast (PC) class, the adaptive optical (AO) class and the in-line (IL) class of BioCD. Of these different quadrature classes, the in-line BioCD has the highest sensitivity with a detection sensitivity of 0.25 pg/mm. The minimum detectable mass is set by simple scaling relations. The metrology limit is set by surface roughness combined with repositioning offset between pre- and post-incubation scans. Optimal sensitivity is achieved by critical sampling of protein spots in radial arrays.

8:24AM H16.00003 Docetaxel-loaded Nanohorn-streptavidin-antibody for Anti-cancer Drug Delivery , JIANXUN XU, MASAKO YUDASAKA, MINFANG ZHANG, JST/SORST, NEC, 34 Miyukigaoka, Tsukuba, Ibaraki 305-8501, SUMIO IIJIMA, Meijo University, Nagoya 468-8502, Japan — Single wall carbon canohorn (SWNH) is a new kind of nano-carbon tubule having horn-like structure at its tip. The tube diameters are 2 to 5 nm, and about 2,000 SWNHs assemble to form a spherical aggregate. SWNH is an attractive candidate for drug delivery, especially promising to carry anticancer drug, many of which are not water soluble and highly toxic. We incorporated Docetaxel (Doc), an anticancer drug used for stomach cancer and others, into hydrogen peroxide treated SWNH (SWNHox). By using carboxylic groups on SWNHox, we attached amine-PEO3-biotin, and then streptavidin to biotin. The streptavidin moiety on SWNH makes it easy to attach some other biotinylated molecules, thus we introduced a cancer targeting ligand, anti-tumor associated glycoprotein, to the SWNH system. Due to the targeting effect of the antibody, the cells were effectively killed when they were incubated with the Doc SWNHox-streptavidin-andtibody system.

8:36AM H16.00004 Detection limits and scalability of miniaturized antibody assays in real-world applications , BRIAN HAAB, Van Andel Institute — Antibody-based analytical assays have increasing importance in biological and biomedical applications. The ability to miniaturize the assays can lead to increased multiplexing and throughtput, thus increasing information content while saving on the consumption of valuable samples and reagents. However, several challenges need to be addressed to enable the implementation of such technologies. This talk will address the factors affecting detection limits and scalability in real-world applications of antibody microarrays for the study of proteins in human blood serum.

9:12AM H16.00005 InAs quantum well μ-Hall sensors for magnetic biosensing , KHALED ALEDEALAT, S. HIRA, K. CHEN, Florida State Univ, G. MIHAJLOVIC, Materials Science Division, Argonne National Lab, P. XIONG, G. STROUSE, P.B. CHASE, S. VON MOLNAR, Florida State Univ, M. FIELD, G. SULLIVAN, Teledyne Scientific Company LLC — Magnetic sensing is potentially a sensitive and rapid technique for monitoring DNA-DNA and protein-DNA interactions. Here we present an effort on the noise characterization and selective biofunctionalization of InAs μ-Hall sensors for magnetic detection of DNA hybridization. Room-temperature noise measurements were performed in the frequency range from 20 Hz to 104 kHz. The noise equivalent magnetic moment resolutions were estimated to be $\sim 10^6 \quad \mu_B/\sqrt{Hz}$ and $\sim 10^4 \quad \mu_B/\sqrt{Hz}$ at 92 Hz and 23 kHz respectively. The active region of the InAs μ-Hall device was covered with sputter-deposited SiO_2 and Au pads were patterned on top of some of the Hall crosses. Thiolated ssDNA were assembled on the Au pads and the rest of the device platform was passivated with PEG-silane. Biotinylated and fluorescently-tagged complementary ssDNA were labeled with commercial streptavidin-coated 350 nm superparamagnetic beads, which were found to assemble selectively onto the Au pads through DNA hybridization using laser scanning confocal microscopy. This work was supported by NIH NIGMS GM079592.

9:24AM H16.00006 Ligand-receptor binding kinetics in surface-plasmon resonance devices: A Monte Carlo simulation study[1] , MATTHEW T. RAUM, Department of Physics, Virginia Tech, Blacksburg, VA 24061-0435, MANOJ GOPALAKRISHNAN, Harish-Chandra Research Institute, Allahabad 211019, India, KIM FORSTEN-WILLIAMS, Department of Chemical Engineering, Virginia Tech, Blacksburg, VA 24061, UWE C. TAUBER, Department of Physics, Virginia Tech, Blacksburg, VA 24061-0435 — We use lattice Monte-Carlo simulations to probe the kinetics of ligand-receptor association and dissociation. Simulations were run under conditions approximating the geometric configuration of surface plasmon resonance devices. These conditions include viscous flow of ligands over a surface of receptors which is achieved by using a spatially varying biased random walk. Our simulations allow for the occurrence of multiple rebinding events which result in strong deviations from the standard mean-field rate equation approximation. Our simulations also allow us to test improved theoretical predictions for the binding dynamics and to determine their range of applicability.

[1]Research in part funded through the National Science Foundation, NSF DMR-0075725.

9:36AM H16.00007 Comparative study of different DNA chip preparation methods by means of Surface Plasmon Resonance , YANNICK SARTENAER, Laboratoire Lasers et Spectroscopies - FUNDP - University of Namur, 61 rue de Bruxelles, B-5000 Namur, Belgium, RYUJI HARA, HARUMA KAWAGUCHI, Laboratory of Polymer Chemistry - Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan, PAUL A. THIRY, Laboratoire Lasers et Spectroscopies FUNDP - University of Namur, 61 rue de Bruxelles, B-5000 Namur, Belgium — Recently, we demonstrated that SFG vibrational spectroscopy allows the detection of the specific recognition between the two molecules of a model ligand-protein biosensor. Moreover, we studied by this technique, the formation of thiolated single stranded DNA (ssDNA) monolayers immobilized on metallic substrates which are the basis for various biotechnology applications. Before going further into monitoring the hybridisation process in DNA based sensors, it is important to identify a preparation method providing good quality DNA chips with respect to the recognition process. Therefore, we performed investigations by Surface Plasmon Resonance (SPR). Practically, we used four different methods of chip preparation on gold surfaces and we measured the amount of deposited molecules when the sensor is exposed to a target DNA solution. By this way, we monitored for each case the sensitivity and the selectivity of the sensor by comparing the hybridisation of complementary and non complementary target ssDNA, respectively.

9:48AM H16.00008 Nanoscale Building Blocks for Biosensor Development , AMANDA J. HAES, Department of Chemistry, University of Iowa — The development of new technologies based on nano- and microscale phenomenon is important and significant for many reasons. One of the most prominent of these is biological sensors for the diagnosis of diseases, detection of environmental toxins, and drug discovery. Research in our group focuses on the microscopic and spectroscopic analysis of the optical properties of nanostructures and their integration with microfluidic devices with applications in biological sciences. In this talk, we will show results for an optical sensor based on localized surface plasmon resonance spectroscopy. It will be demonstrated that this nanoparticle based sensor can be used to detect a variety of ligands, including a biomarker for Alzheimer's disease.

10:24AM H16.00009 Predictive Model for Label-free Electrical Detection of Bio-molecules , PRADEEP NAIR, MUHAMMAD ALAM, School of Electrical and Computer Engineering, Purdue University — Biosensors based on MOSFETs, silicon nanowires, and carbon nanotube nanocomposites *promise* highly sensitive, dynamic, label-free, electrical detection of bio-molecules with potential applications in genomics and proteomics. Although tremendous improvements in sensitivity have been reported in electrical detection of bio-molecules, many aspects of experimentally observed sensor response (S) are unexplained within the theoretical frameworks of kinetic response or electrolyte screening. In this paper, we combine analytic solutions of Poisson-Boltzmann and reaction-diffusion equations to show that the electrostatic screening within an ionic environment limits the response of nanobiosensor such that $S(t) \sim c_1 \left(\ln(\rho_0) - \frac{\ln(I_0)}{2} + \frac{\ln(t)}{D_F} + [pH] \right) + c_2$ where c_i are geometry-dependent constants, ρ_0 is the concentration of target molecules, I_0 the salt concentration, and D_F the fractal dimension of sensor surface. Our analysis provides a coherent theoretical interpretation of wide variety of puzzling experimental data that have so far defied intuitive explanation and have important implications for the design and optimization of nanoscale biosensors.

10:36AM H16.00010 Hybrid CMOS/Microfluidic Dielectrophoresis and Magnetic Manipulator Chip[1] , DAVID ISSADORE, Harvard School of Engineering and Applied Sciences (SEAS), THOMAS P. HUNT[2], Harvard Physics, KEITH A. BROWN, Harvard SEAS, R.M. WESTERVELT, Harvard SEAS and Physics — We present hybrid CMOS/microfluidic chips that combine the biocompatibility of microfluidics with the programmability of CMOS integrated circuits (ICs). The chips use a two-dimensional array of RF-electrode pixels that use dielectrophoresis (DEP) to simultaneously and independently control the location of many objects, including biological cells and chemical droplets [1]. We highlight our next generation of CMOS/microfluidic chips that combine a two-dimensional array of high voltage (50 V) RF pixels to produce large DEP forces, a microelectromagnetic matrix [2] that can independently trap and move magnetic beads, and integrated temperature sensors. We show the design, fabrication, and testing of the hybrid chips as well as ongoing work to interface and package the chips for robust biological and chemical experiments. [1] T.P. Hunt, D. Issadore, R.M. Westervelt, Lab Chip, 2008, DOI: 10.1039/b710928h. [2] H. Lee, A.M. Purdon and R.M. Westervelt, Appl. Phys. Lett. 85, 1063 (2004).

[1]Supported by the NCI MIT-Harvard CCNE [1U54CA119349] and by the DoD through the NDSEG Fellowship Program
[2]Currently at UC Berkeley Bioengineering

10:48AM H16.00011 Hybrid CMOS/Microfluidic Chip Applications[1] , KEITH A. BROWN, DAVID ISSADORE, Harvard University School of Engineering and Applied Science, THOMAS P. HUNT[2], Harvard University Department of Physics, R.M. WESTERVELT, Harvard University School of Engineering and Applied Science, Harvard University Department of Physics — We present our continuing work on hybrid CMOS/microfluidics systems that enable programmable experiments on single biological cells and picoliter chemistry. A 128x256 array of 10x10 micron RF-electrode pixels in the integrated circuit (IC) allows positioning of cell-sized objects using dielectrophoresis in a microfluidic chamber observed using a fluorescence microscope[1]. The fluid environment in the chamber is controlled through external piping, integrating the hybrid chip into a complete microfluidic system. We demonstrate the use of this integrated circuit as a cell-sorting stage. Applications and prototypical experiments with relevance to biologically motivated research will be presented. We highlight single cell experiments made possible by the ability to move, combine and separate picoliter droplets using computer control with video feedback. [1] Thomas P. Hunt, et al. Lab Chip, 2008, DOI: 10.1039/b710928h

[1]Supported by the NCI MIT-Harvard CCNE [1U54CA119349] and by the DoD through the NDSEG Fellowship Program.
[2]Currenty at UC Berkeley Bioengineering Department

Tuesday, March 11, 2008 11:15AM - 2:03PM –
Session J8 DFD GSNP: Granular Flows Morial Convention Center RO6

11:15AM J8.00001 Washboard Road: The dynamics of granular ripples formed by rolling wheels , NICOLAS TABERLET, ANNE-FLORENCE BITBOL, ENS Lyon, France, STEPHEN MORRIS, University of Toronto, JIM MCELWAINE, University of Cambridge — We report laboratory experiments on rippled granular surfaces formed under rolling wheels. Ripples appear above a critical speed and drift slowly in the driving direction. Ripples coarsen as they saturate, and exhibit ripple creation and destruction events. All of these effects are captured qualitatively by 2D soft particle simulations in which a disk rolls over smaller disks in a periodic box. The simulations show that compaction and segregation are inessential to the ripple phenomenon. We describe a simplified scaling model which gives some insight into the mechanism of the instability.

11:27AM J8.00002 Evolution of sand ripples in pulsed flow , JOSÉ EDUARDO WESFREID, CNRS, JOACHIM KRUITHOF, PMMH - CNRS — We present high-resolution experiments showing the temporal evolution of sand ripples formed by oscillatory flow. We discuss the decompaction process observed during the formation of the ripples pattern. We have also studied the evolution of different parameters during the transition of rolling grain ripples to vortex ripples, as the slope of these ripples and we tested the validity of the Sleath criterion to discriminate the transition.

11:39AM J8.00003 Granular Erosion of Pebbles , ADAM ROTH, DOUGLAS DURIAN, University of Pennsylvania — Flowing grains are strongly abrasive, and cause erosion both of themselves and their surroundings. In a geophysical setting, the erosion of pebbles has traditionally been quantified by global measures such as aspect ratio. Recently we have focused on curvature, and its distribution around the contour, as a local measure more directly related to the microscopic action of erosion. Here we apply this method to linoleum shapes, eroded by rotation in an abrasive grit. Several shape parameters are measured at different stages in the erosion process, including the curvature distribution. A simple model of erosion is developed, and its predictions are compared to the data. The results are in reasonable agreement, and could be useful for understanding natural erosion processes.

11:51AM J8.00004 Impact and Penetration of Granular Materials by Discrete Element Simulations , JUSTIN W. GARVIN, Air Force Research Lab, JEREMY B. LECHMAN, J. MATTHEW D. LANE, Sandia National Labs — Granular material response to impact is important in a range of fields, from munitions delivery, to meteorite collision and crater formation. Recently a model for the force experienced on a penetrator has been proposed [L.S. Tsimring and D. Volfson, Powders and Grains 2005, 1215-1223] and shown to fit experimental data well [H. Katsuragi and D.J. Durian, Nature Physics, Vol. 3, June 2007]. This model describes two components of the force: i) a velocity dependent, depth independent term related to the inertial force required to mobilize a volume of grains in front of the penetrator; and ii) a velocity independent, depth dependent, Coulomb friction-like term. In the current study, massively parallel, discrete element simulations have been performed to study the penetration of a large spherical impactor into a multi-million particle bed of granular material. Results agree with previous work for slow impact speeds ($<$ 400cm/s). In addition, the current work extends the comparison with the proposed model to higher speeds ($\sim$1000cm/s). The physics of the phenomenon is discussed along with the challenges for modeling and simulation in the even higher velocity regime.

12:03PM J8.00005 Gas-Mediated Impact Dynamics in Fine-Grained Granular Materials[1] , JOHN ROYER, ERIC I. CORWIN, BRYAN CONYERS, MARK L. RIVERS, PETER J. ENG, HEINRICH M. JAEGER, James Franck Institute, University of Chicago — Non-cohesive granular media exhibit complex responses to sudden impact that often differ from those of ordinary solids and liquids. We investigate how this response is mediated by the presence of interstitial gas between the grains. Using high-speed x-ray radiography we simultaneously track the motion of a steel sphere through the interior of a bed of fine-grained granular material and measure local changes in the bed packing density below the sphere. In an initially loosely packed bed, interstitial gas allows for nearly incompressible, fluid-like flow of the bed and aids the penetration of the sphere. In an initially densely packed bed the interstitial gas plays the opposite role, strengthening the bed and inhibiting the penetration of the sphere. These two seemingly incongruous effects are both due to the low permeability of the fine grained-bed, which traps the interstitial gas in the bed. This trapped gas resists changes in the bed packing density, inhibiting compaction in the loose bed and inhibiting dilation in the dense bed.

[1]This work was supported by NSF through DMR-MRSEC and by DoD/AFSOR.

12:15PM J8.00006 Impact cratering in fluidized granular matter , PATRICK MAYOR, HIROAKI KATSURAGI, DOUGLAS J. DURIAN, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — Impacts by projectiles dropped into granular media are an important example of how particulate materials respond to externally applied forces. Beyond the obvious geophysical case of planetary craters, understanding the details of impact mechanisms can provide valuable information on these systems, and the phenomenon has been actively investigated. In particular, recent experiments have studied the penetration depth of projectiles impacting granular materials at relatively low speeds, and measured the dynamics of the impact process, yielding force laws accounting for the observations. We have studied how the impact phenomenon is affected when the granular medium is submitted to a vertical upward (or downward) gas flow, in a range of flow rates below the bubbling regime. These fluidized granular systems yield, logically, deeper impacts, and dynamics measurements reveal that the stopping time is also longer, contrary to what is observed when deeper craters are obtained by increasing the impact velocity. We observe that the parameters involved in previously obtained force laws are modified in a simple way as a function of the flow rate and find a velocity-dependent inertial term and a depth-dependent friction force that vanishes as the flow rate approaches the fluidization threshold.

12:27PM J8.00007 Drag Force in a Gas Fluidized Granular Bed , T.A. BRZINSKI, D.J. DURIAN, University of Pennsylvania, Dept. of Physics — We use a rheometer to measure the torque acting on a rotating bar in a bed of gas-fluidized glass beads. We vary rotation rate from .001-10rps, vary depth from 1-10 cm, and increase the fluidizing gas flow from no flow well into the fluidized regime. We observe that at high rotation rates the drag is roughly proportional to velocity squared. At low rates we can rescale the measured torque by depth, and observe a collapse of the data. These results agree with the predictions of a granular drag force model which has proven effective in predicting granular impact dynamics. The model consists of an inertial drag term, which is depth-independent and scales as velocity squared, and a frictional drag term, which is independent of rate and varies linearly with depth. We find, as expected, that while the frictional term is airflow-dependent the inertial term is uncoupled from the fluidization.

12:39PM J8.00008 Exploring penetration through granular media , DANIEL J. COSTANTINO, Department of Physics; Pennsylvania State University, THOMAS J. SCHEIDEMANTEL, MATTHEW B. STONE, JULIA COLE, CASEY CONGER, KIT KLEIN, MATTHEW LOHR, WILLIAM MCCONVILLE, ZACHARY MODIG, KRYSTEN SCHEIDLER, PETER SCHIFFER — The motion of objects through granular media is an important physical problem involving local jamming of the grains. We report on an experiment dealing with the force needed to initiate upward motion through a granular pile, F_{ini}. As expected, this force scales monotonically with the depth of the intruder as well as its size, D_{plate}. However, unlike previous experiments this force also depends on the size of the particles making up the pile, d_{grain}. The force can be represented by the function $F_{ini} = AD_{plate} \quad d_{grain} + BD^2_{plate}$; which can be qualitatively explained within a simple model. Finally, preliminary results from a new experiment dealing with horizontal motion through a granular pile will be discussed. In this study, the effect of interstitial fluids on a granular material's resistance to an intruder will be investigated. Research supported by NASA grant NAG3-2384 and the NSF REU program.

12:51PM J8.00009 Fluctuations in an agitated granular fluid , KIRI NICHOL, MARTIN VAN HECKE, Leiden University — Granular media can be fluidized by a flow that occurs far away. Intruders placed in such a 'stationary granular fluid' sink until they reach a depth given by a granular analogue of Archimedes law. Once they float at this depth, these intruders effectively probe the microscopic agitations in the material that cause the fluidization. The spectrum of these fluctuations is anomalous. We present its dependence on experimental parameters such as driving rate, floating depth and probe size, and discuss the possibility of applying a non-equilibrium Fluctuation Dissipation relation to this system.

1:03PM J8.00010 Jamming in Hopper Flow of Large Aspect Ratio Granular Materials , SCOTT FRANKLIN, Rochester Institute of Technology — The clogging of granular materials at the exit of a silo or hopper is a matter of tremendous practical importance, as well as a canonical example of jamming. We investigate the effect of particle aspect ratio (length:width) on the jamming probability through experiments and discrete element simulations. Preliminary experimental results on particles with aspect ratios of 16 and 32 show that the probability $P(m)$ for m grains to exit the hopper has an exponentially decaying tail that, when scaled by the mean number that exit, is independent of exit aperture size. This scaling of $P(m/\langle m \rangle)$ is also observed in hopper flow of ordinary round materials, but the proposed phenomenological explanation of uncorrelated behaviors seems unlikely in long, thin rods. Furthermore, while the mean exit number obviously increases with aperture size, it is not clear which length scale is most relevant: particle length, width, or some combination of the two. We are also writing new discrete element simulations that can be compared with the experiments, and I will discuss some of the computational nuances introduced by particle asymmetry and present initial results.

1:15PM J8.00011 Granular Flow of Fluid-Submerged Particles: Effects of Fluid Viscosity , H. KING, D. ERTAS, A. KUSHNICK, F. ZHOU, ExxonMobil, P. CHAIKIN, NYU — Gravity-driven flows of granular materials are often influenced by interstitial fluids. Using the rotating half-filled drum geometry, we investigated particle and fluid velocities for granular flows of nearly monodisperse spherical glass particles with interstitial fluids of varying dynamic viscosity (air to 4 cP). We utilize direct particle imaging and PIV methods. For dry flows the fundamental time scale is set by the gravitational constant and particle size. We observe two primary influences of the interstitial fluid on the granular rheology. First, density of the fluid changes both the driving force (due to buoyancy) and the inertial response (due to added mass), increasing the characteristic time scale. Second, the intrinsic time scale is influenced by the dynamic viscosity of the fluid. As a result, the changes associated with the 1 cP viscosity increase in going from air-to-water are considerably larger than those for subsequent viscosity increments. We also see that the surface drag associated with the fluid boundary layer progressively affects the grain velocity profile near the surface as the viscosity increases, giving a several-particle-deep zone of constant velocity.

1:27PM J8.00012 Rheology and structure of granular flows in split-bottom geometries. , JOSHUA DIJKSMAN, MARTIN VAN HECKE, Leiden University — Combining rheological methods with surface flow imaging, we probe the flow of slow dry granular media as function of driving rate and geometry. The flow rate affects the spatial structure of the flow much stronger than the stresses, while details of the boundary conditions significantly modify both stresses and flow. We discuss our results in the context of recent numerics on rapid flows in these split-bottom geometries, and various theories developed for slow flows.

1:39PM J8.00013 Self-diffusion in bulk sheared granular materials , ANDREEA PANAITESCU, ASHISH ORPE, ARSHAD KUDROLLI, Department of Physics, Clark University — We will discuss the diffusion and structural properties of granular particles in the bulk of a cyclically sheared three dimensional rectangular cell. The particles are visualized away from the side walls using a fluorescent refractive index matched interstitial fluid. Previous studies have shown that the diffusion is anisotropic with respect to the vorticity plane, but these results have been confined to either two dimensional systems or small three dimensional systems where the boundary effects could not be decoupled. In a cyclic shear cell, the packing fraction the particles and their orientational order vary smoothly over time. The particle positions are identified and tracked over long durations to obtain particle diffusivity, mean-squared displacements and probability distributions of particle displacements. An analysis of the effect of structural order on the motion of the particles will be presented.

1:51PM J8.00014 Studies in a 2D granular pure shear experiment , JIE ZHANG, Department of Physics and CNCS, Duke University, NC 27708, USA, PEIDONG YU, TRUSH MAJMUDAR, ROBERT P. BEHRINGER — We have performed two dimensional granular experiments under pure shear using bidisperse photo-elastic disks. Starting from a stress free state, a squre box filled with granular particles is subject to shear. The forward shear involved thirty steps, leading to maximum strain of 0.1. The network of force chains gradually built up as the strain increased, leading to increased pressure and shear stress. Backward shear was then applied to return the system to zero strain in the next thirty steps. Following each change of the system, contact forces of individual disks were measured by applying an inverse algorithm. We also kept track of the displacement and angle of rotation of every particle from frame to frame. We present the results for the contact forces, particle displacement, particle rotations, fabric, etc. Work supported by NSF grant DMR0555431.

Tuesday, March 11, 2008 11:15AM - 1:27PM –

Session J9 DFD: Fluid Structure and Properties Morial Convention Center RO7

11:15AM J9.00001 The Interplay of Short- and Long-Ranged Forces in Simulations of Confined Water using Local Molecular Field Theory , JOCELYN RODGERS, JOHN WEEKS, University of Maryland, College Park — A molecular model of water confined between walls is studied using local molecular field (LMF) theory. LMF theory splits the long-ranged Coulomb $1/r$ potential between charge sites into a short-ranged core potential and a long-ranged, slowly-varying potential ideal for mean-field averaging. The core potential may be treated explicitly by simulations using the minimum image convention with a renormalized external field defined by mean field averaging of the longer-ranged potentials. Here we apply local molecular field theory to molecular dynamics simulations of molecular water confined between walls, with and without an electric field. This is a geometry where short-ranged spherical truncations of Coulomb interactions can fail spectacularly, but in tandem with the effective external field defined by LMF theory such truncations correctly predict structural and electrostatic properties of water. Further the concepts behind LMF theory elucidate the varying contributions of hydrogen-bonding and dipolar interactions in determining the structure of water at surfaces.

11:27AM J9.00002 Effects of a solute on a simple model solvent[1] , PAOLO DE GREGORIO, JONATHAN C. TOLEDO, B. WIDOM, Department of Chemistry, Baker Laboratory, Cornell University, Ithaca NY, USA — We studied the effect of the addition of a solute on a one-dimensional model solvent (high density, low compressibility, low coefficient of thermal expansion), at infinite dilution. The solute has a solubility which is low and decreases with increasing temperature. The effect of the addition of solutes on the chemical potential of the solvent at constant volume differs from that at constant pressure in a way similar to that of non-polar solutes in water. The solvent-solvent pair distribution function determines fully the modes of decay of the solute-solute counterpart. At the largest distances, the ultimate decay is strictly monotonic (exponential) for both. But while for the solvent-solvent correlations the amplitude associated with that mode is negligible, it is huge for the solute-solute case. Formally, the correlations vanish in identical fashion at infinite distances, but they differ substantially over an extended range of physical interest. The osmotic second virial coefficient is very large and negative, not only as an effect of the proximity 'attraction' between the solutes, but also of the very long tail in the correlations.

[1]NSF support is acknowledged.

11:39AM J9.00003 Ultrafast Phase-Contrast Imaging Study of Finite-time Hydrodynamic Singularities , YUJIE WANG, Argonne National Lab — Most of the nonlinearity induced hydrodynamic singularities are transient and requires high-speed imaging to be studied. There exist some intrinsic problems of visible-light imaging on fluid mechanical research.. The key advantage of x-ray phase-contrast-imaging is that it is interface-based technique and the boundaries are highlighted naturally. It is a highly penetrative technique in which all complex structures along the path will be picked up. Additionally, it is naturally immune of the complexity of multiple scattering and strong optical reflection or refraction.

11:51AM J9.00004 Liquid State Properties from *ab initio* Density Functional Theory Calculations , NICOLAS BOCK, TRAVIS PEERY, ERIC CHISOLM, GIULIA DE LORENZI-VENNERI, DUANE WALLACE, Los Alamos National Laboratory, ERIK HOLMSTRÖM, RAQUEL LIZARRAGA, Instituto de Fisica, Universidad Austral, Chile — For the solid state, density functional theory (DFT) has been successfully applied to calculate material properties in a large range of materials. In the liquid state however, thermodynamic properties are calculated by molecular dynamics (MD) simulations in which the forces are calculated with DFT. These simulations are computationally significantly more expensive than comparable solid state calculations. We present a novel approach which does not rely on MD simulations, but instead uses Vibration-Transit (V-T) theory to make predictions of the thermodynamic properties of the liquid phase. This approach is computationally significantly less expensive than an MD simulation. The accuracy of this approach is demonstrated by a comparison to experiment.

12:03PM J9.00005 Reconstructing the structure and dynamics of density fluctuations in water near a moving proton , ROBERT CORIDAN, GHEE HWEE LAI, NATHAN SCHMIDT, Department of Physics, University of Illinois, Urbana-Champaign, PETER ABBAMONTE, Department of Physics and Seitz Materials Research Lab, University of Illinois, Urbana-Champaign, GERARD C. L. WONG, Department of Materials Science Engineering, Department of Physics, and Seitz Materials Research Lab, University of Illinois, Urbana-Champaign — The structure and dynamics of water on femtosecond timescales is relevant to many topics in physical chemistry such as ion solvation. We computationally reconstruct the angstrom-scale spatial and femtosecond-scale temporal evolution of density fluctuations in water using high-resolution inelastic x-ray scattering (IXS). The imaginary part of density propagator $\chi(\mathrm{q},\omega)$ is directly extracted from the IXS data, and the real part recovered using Kramers-Kronig relations. The resultant complex-valued $\chi(\mathrm{q},\omega)$ is the Fourier transform of the real-space density-density response function $\chi(\mathrm{r},\mathrm{t})$ which measures the dynamical density fluctuations of water due to a point-like instantaneous pulse. We use this density propagator from IXS data and linear-response theory to reconstruct the hydration behavior of a proton moving at different speeds through water.

12:15PM J9.00006 Classical Density Functional Theory of Inhomogeneous Polar Molecular Liquids , JOHANNES LISCHNER, T.A. ARIAS, Cornell University — We show how free energy functionals for classical assemblies of interacting rigid molecules, composed of an arbitrary number of atoms, can be constructed, such that the entropy of the noninteracting assembly, the thermodynamic properties and the microscopic order of the uniform phase and the dielectric properties in both weak and strong electrostatic fields are reproduced. We use our approach to predict density profiles of liquid hydrogen choride in a parallel plate capacitor with different wall potentials and varying external fields. We show that our theory can easily be coupled to electronic structure calculations within the Joint Density Functional approach and will comment on potential application to water.

12:27PM J9.00007 Localized Voronoi analysis of quenched liquid configurations , TRAVIS PEERY, NICOLAS BOCK, GIULIA DE LORENZI-VENNERI, DUANE WALLACE, Theoretical Division, Los Alamos National Laboratory, ERIK HOLMSTROM, Instituto de fisica, Universidad Austral de Chile — We developed a set of *localized* statistical tools to explore and characterize condensed matter particle configurations, particularly amorphous distributions associated with the liquid state. Typically global measures of atomic packing are used to characterize atomic configurations, such as pair distribution functions. For large systems, such calculations can be computationally expensive and tend not to be sensitive to localized symmetries. Our localized tools are based upon the geometric or topological analysis of (static) atomic arrangements using Voronoi polyhedra. As each atom in the configuration has a unique Voronoi polyhedron defined by its near neighbors, our tools can describe the geometry and symmetry of local neighborhoods. We have defined, for example, a local, Shannon-type entropy for the Voronoi coordination number for each atom in a 500-atom, monatomic system. This *localized* entropy tool was able to find small (9–40 atom) crystallites or regions of high symmetry in an otherwise random 500-atom configuration quenched from a liquid MD state. These tools will help to define and characterize not only random liquid state configurations and the minimum structures associated with liquid potential energy surfaces, but also the symmetry properties of the quenching process itself.

12:39PM J9.00008 Phase Separation in the Dipolar Hard-Sphere System Revisited[1] , WONKI ROH, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — We investigate the liquid-vapor transition in the dipolar hard-sphere system. Since the suggestion of de Gennes and Pincus [Phys.Kondens. Mater. **11**, 189 (1970)] this phase transition has proven both elusive and controversial, with conflicting numerical results regarding its existence and its nature. Employing extensive and efficient grand-canonical Monte Carlo simulations, we revisit this issue. High-precision results on the low-temperature heat capacity are presented along isotherms as well as isochores. In addition, we study the density distribution function and its moments for a wide range of chemical potentials, and identify anomalous finite-size effects that can give rise to incorrect conclusions.

[1]This work was supported by the U.S. Department of Energy under Grant No. DE-FG02-07ER46471.

12:51PM J9.00009 X-ray tracer study of Rheology and Hydrodynamics of Fatty acids , MENGNING LIANG, University of Illinois at Urbana Champaign, ROSS HARDER, IAN ROBINSON, University College London, UNICAT TEAM — In wormlike micelles, the breaking and reforming of the micelle rods and the shearing of the rods and between the carbon chains themselves result in a complex diffusive behavior with more than one characteristic time constant. This is one of the characteristics of a Maxwellian fluid. We have studied the rotational Brownian motion of an alumina crystal suspended in a fatty acid liquid. Synchrotron generated hard x-rays are used to do single particle tracking of the rotational orientation by tracking the Bragg intensity of alumina crystals in diffraction geometry. This technique allows the tracking of particles to sub-milliradian precision. We have observed multiple time scales of relaxation which is evidence of subdiffusive behavior.

1:03PM J9.00010 Statics and dynamics of a cylindrical droplet under an external body force , JAMES SERVANTIE, MARCUS MÜLLER, Institute For Theoretical Physics, Goettingen — We study the rolling and sliding motion of droplets on a corrugated substrate by Molecular Dynamics simulations. Droplets are driven by an external body force (gravity) and we investigate the velocity profile and dissipation mechanisms in the steady state. The cylindrical geometry allows us to consider a large range of droplet sizes. The velocity of small droplets with a large contact angle is dominated by the friction at the substrate and the velocity of the center of mass scales like the square root of the droplet size. For large droplets or small contact angles, however, viscous dissipation of the flow inside the volume of the droplet dictates the center of mass velocity that scales linearly with the size. We derive a simple analytical description predicting the dependence of the center of mass velocity on droplet size and the slip length at the substrate. In the limit of vanishing droplet velocity we quantitatively compare our simulation results to the predictions and good agreement without adjustable parameters is found.

1:15PM J9.00011 Velocity-dependent friction coefficient at the interface between a polymer melt and a solid substrate , NIKOLAI PRIEZJEV, ANOOSHEH NIAVARANI, Michigan State University — Molecular dynamics simulations are carried out to investigate the dynamic behavior of the slip length in thin polymer films confined between atomically smooth thermal surfaces. For weak wall-fluid interactions, the shear rate dependence of the slip length acquires a distinct local minimum followed by a rapid growth at higher shear rates. With increasing the fluid density, the position of the local minimum is shifted to lower shear rates. We found that the ratio of the shear viscosity to the slip length, which defines the friction coefficient at the liquid/solid interface, undergoes a transition from a nearly constant value to the power law decay as a function of the slip velocity. In a wide range of shear rates and fluid densities, the friction coefficient is determined by the product of the value of surface induced peak in the structure factor and the contact density of the first fluid layer near the solid wall. A relation to recent slip flow experiments is discussed. Reference: A. Niavarani and N.V. Priezjev, Phys. Rev. E (2008) (cond-mat/0711.0178).

Tuesday, March 11, 2008 11:15AM - 2:15PM –

Session J16 DBP DFD: Focus Session: Biochip Physics II Morial Convention Center 208

11:15AM J16.00001 Direct-Print Organic Photonics for Biodetection Chips , MAX SONNLEITNER, BIOIDENT Technologies Inc. — The development of commercial portable Biochip applications based on optical detection is hindered by the lack of imaging systems that can be directly integrated into the chip itself. Currently, fluorescence/luminescence signals are read out with power-hungry, bulky and expensive off-chip imaging systems, like CCD cameras or photomultiplier tubes. Here we present an enabling technology that for the first time allows cheap and easy integration of imaging systems directly into disposable Biochip systems. Our technology is based on organic semiconductor materials that can be processed in liquid form by inkjet and screen printing, in a process much faster and cheaper than the complicated fabrication of silicon-based imaging sensors. Organic photosensors can be printed on various substrate materials like plastic foil or glass or directly onto Biochip systems. The ultrathin photodiodes with an overall thickness of only 300 to 500 nm show quantum efficiencies better than 0.5 and linear light-response over 6 orders of magnitude. The pixel size can range from 50 to over 1000 μm and inkjet fabrication allows tailoring the sensor layout to the needs of the specific application. Single photodiodes, photodiode line-arrays or 2D arrays of photodiodes can be printed onto diverse materials. Besides the dramatically reduced production costs for printed photodiodes, the presented readout architecture allows detection of e.g. chemiluminescence signals with highest sensitivities and minimum crosstalk due to the close proximity of sample and printed photodiode.

11:51AM J16.00002 On-the-flow differentiation between cells based on native fluorescence spectroscopy on a chip , MARKUS BECK, MICHAEL BASSLER, PETER KIESEL, NOBLE M. JOHNSON, OLIVER SCHMIDT, Palo Alto Research Center, 3333 Coyote Hill Rd, Palo Alto, CA 94034 — Native fluorescence spectroscopy is a promising approach for the detection of pathogens without specific binding or tagging of the analyte. The distinction between different species is possible with (multi-color) UV excitation together with the detection of several spectral bands. We have developed a compact platform that combines a microfluidic quartz channel with chip-size wavelength-selective detection of the fluorescence from particles traversing the channel. The interaction between the UV excitation light and the analyte is enhanced by anti-resonantly guiding the light within fluid. We have recorded the intrinsic fluorescence of single cells (e.g. yeast, e-coli, and BT) passing the detection area. Knowing the particle speed and the physical dimensions of the observation window, we are able to determine particle positions with microscopic ($\sim$10 microns) resolution. A special modulation technique allows us to achieve a high signal to noise ratio even for high particle speeds. Combining our technique with a cell sorting mechanism would allow for on-the-chip characterization and sorting of untagged cells.

12:03PM J16.00003 Design of a Molecular Diode: Nanoratchets[1] , ROBERT AUSTIN, JASON PUCHALLA, PETER GALAJDA, KEITH MORTON, Princeton University — We use the concepts hydrodynamic flow in asymmetric structures and apply them to our own asymmetric bump array/diffusion array technology at the nanoscale. Our basic premise is that asymmetrically designed metamaterials at the nanoscale can act, under the influence of externally applied forces, as molecular ratchets which will sort molecules based on their size. At some nano length scale, we believe that the classical concepts of stick boundary conditions break down and a new regime of transport begins. We present computer simulations and experiments which show that at the nanoscale level we can efficiently separate objects the size of proteins.

[1]Supported by DARPA grant W911NF-05-1-0392

12:15PM J16.00004 Toward on-chip directed evolution of unicellular organisms for efficient hydrogen production[1] , DAVID LIAO, CALEB HOWE, CECILIA MULDOON, PETER GALAJDA, JUAN KEYMER, ROBERT AUSTIN, Princeton University — To provide an energy resource alternative to fossil fuels, photosynthetic organisms must increase their energy conversion efficiency. The green algae *C. reinhardtii* stores light energy in hydrogen gas at 0.1% efficiency, less than the 10% required to compete with established fuels. This work combines hydrogen sensing in liquid culture with micro habitat patch (MHP) chips for directing hydrogen-producing organisms to evolve improved energy conversion efficiency. A MHP chip contains 87 1 mm $\times$ 1 mm $\times$ 100 μm interconnected chambers. By measuring hydrogen output from different chambers, we will select less productive patches to annihilate. We microfabricated chips from poly(dimethylsiloxane). Color changes in fluorescence micrographs confirm that 254 nm radiation kills algae in MHPs, liberating nutrients and space for exploitation by adjacent populations. We demonstrated colorimetric detection of hydrogen gas production at a rate of 10^{-8} mol H_2 mL^{-1} s^{-1} using tungsten film on sub-mL liquid cultures of *C. reinhardtii* during 2-hrs. of fermentation in darkness.

[1]BioSolar H2 AFOSR MURI FA9550-05-1-0365

12:27PM J16.00005 Rapid Detection of Microorganisms–State of Art and Future Directions , GEORGE HONG, Millipore Corporation — For the last several decades, nutrient-based culture growth methods have been accepted as the standard for microorganism detection and identification. However, since the discovery of nucleic acids and molecular breakthrough technologies such as restriction enzymes and polymerase chain reactions, the detection and identification of microorganisms have advanced to culture-independent methods that fall under the category of rapid microbial detections. Here, we present an overview of major rapid microbial detection technologies. These technologies will include both amplification and non-amplification based methods for the detection and identification of target microorganisms. The technologies described can be applied to detecting a wide variety of microorganisms, including bacteria, viruses, mycoplasma, and fungi and have the potential sensitivity to detect a single microorganism. Also in this presentation, we will present examples of real-life applications as well as future challenges for the advancement of the field of rapid microbiology.

1:03PM J16.00006 Guidance and detection of neuronal cells using Si nanomembranes[1] , CRISTIAN STAII, WEINA PENG, HYUK JU RYU, DON E. SAVAGE, YU HUANG, SOOKIN NAM, JUSTIN WILLIAMS, ERIK DENT, MAX G. LAGALLY, SUSAN N. COPPERSMITH, MARK A. ERIKSSON, University of Wisconsin, Madison — "Lab-on-a-chip" microfluidic technology [1] has emerged as a powerful tool for studying biological systems. Unlike standard macro-scale systems used for decades, microfluidics allows the micro-environment of a neuronal cell culture to be finely regulated. The reduction in feature sizes gives control over fluid phenomena such as laminar flow, shear stresses, and velocity profiles. Here we present a new approach to "lab-on-a-chip" design for studying neuronal cells, integrating microfluidic systems with silicon nanomembrane-based microelectronics. We show that this technology permits rapid production of microchannels with a large variety of shapes/sizes, thereby allowing the exposure of neuronal cell cultures to multiple environments, both mechanical and chemical, simultaneously. In addition, these microfluidic channels can be easily integrated with silicon nanomembrane based electronics. [1] A.J.Blake, T.M.Pearce, N.S.Rao, S.M.Johnson and J. C. Williams, Lab Chip, 2007, 7, 842.

[1]Work supported by: DOE, NSF, NIH-NINDS

1:15PM J16.00007 Well-Oriented NanoWell Array Metrics for Digital NanoBioChip , HEAYEON LEE, BONGKUK LEE, TOMOJI KAWAI, The Institute of Scientific and Industrial Research (ISIR-SANKEN), Osaka University, THE INSTITUTE OF SCIENTIFIC AND INDUSTRIAL RESEARCH (ISIR-SANKEN), OSAKA UNIVERSITY TEAM — Recently many researchers have sought new paradigm for nanobiochip that can be miniaturized and integrated to produce intelligent analysis systems in numerous biotechnology. We have been tried to develop biocompatible materials based nanopatterning, self-assembly array to address challenging problem in nanobioscience. In this time, we describe the nanometrics geometry of a well-oriented nanowell (ONW) array derived from nanofabrication technology which can easily be employed for digital detection with a high S/N ratio, miniaturization, integrated assays and single molecule analysis. We fabricated the self-organized nanopatterning of copolymer as a platform of biomolecular nanoarry using nanolithography. We also present a strong specific antibody-antigen interaction on lipid-membrane modified gold surface using ONW. We believe these findings can be related to various nanobiochip applications. References 1. H.Y. Lee, T. Kawai, K.Y.Suh et al, Advanced Materials, In press (2007). 2. H.Y. Lee, T. Kawai et al, Appl. Phys. Lett. 89, (2006) 113901.

1:27PM J16.00008 Magnetically Directed Cell Co-Localization for Cell-Cell Interaction Studies , EDWARD FELTON, DANIEL REICH, Dept. of Physics and Astronomy, Johns Hopkins University, CHRISTOPHER CHEN, Dept. of Bioengineering, University of Pennsylvania — The ability to create ordered patterns of cells has enabled new approaches to various areas of biological interest, such as tissue engineering, biosensing, and the study of interactions between cells. In this work, we apply forces to cells through binding with magnetic nanowires. The nanowires feature high remanent magnetization, allowing for effective manipulation in low-strength magnetic fields, and when used in conjunction with lithographically patterned magnetic microstructures can precisely position cells into predetermined locations. Chemical functionalization then confines the cells to these substrate areas. We have used this technique to create large numbers of isolated pairs of cells by magnetically guiding them to sites on cobalt and permalloy arrays. Further, the use of two different cell types leads to arrays with heterotypic cell pairs in numbers that exceed those attainable with random cell seeding. Initial experiments applying this magnetic cell trapping technique to perform biological studies of cell-cell interactions will also be described.

1:39PM J16.00009 Electromagnetic Sensors of Biological Motors[1] , JIE FANG, K. RAJAPAKSHE, D. PADMARAJ, H. INFANTE, V. VAJRALA, G. MERCIER, W. WIDGER, W. WOSIK, J. MILLER — Biological motors operate on time scales that readily couple to oscillatory electric fields. Modest ac fields applied to cells in an aqueous medium lead to greatly enhanced fields across the plasma membrane or (at kHz frequencies) internal membranes. Membrane complexes thus contribute to both linear and nonlinear responses to sinusoidal fields. For example, activity of motors in mitochondrial and (for chloroplasts) photosynthetic electron transport chains correlate with frequency-dependent second and third harmonics. Our electrode-based biosensors are scalable for micro- and nano-fluidic biochips. At low frequencies (less than 100Hz) we find it advantageous to use SQUIDs, which reduce contact effects and could lead to clinical applications.

[1]The authors acknowledge support by R21CA122153 from NHLBI & NCI, NIH, & from NSF, by the Welch Foundation (E-1221), and by TcSUH.

1:51PM J16.00010 Single-molecule stochastic sensors for proteins using engineered nanopores[1] , LIVIU MOVILEANU, Syracuse University — We were able to design an unusual temperature-responsive pore-based nanostructure with a single movable elastin-like-polypeptide (ELP) loop. If a voltage bias was applied, the engineered pore exhibited transient current blockades, the nature of which depended on the length and sequence of the inserted ELP. These blockades are associated with the excursions of the ELP loop into the nanopore. At low temperatures, the ELP is fully expanded and blocks the pore completely, but reversibly. At high temperatures, the ELP is dehydrated and structurally collapsed, thus enabling a substantial ionic flow. Acidic binding sites comprised of negatively-charged aspartic acid residues, engineered within the pore lumen, produced dramatic changes in the functional properties of the nanopore, catalyzing the translocation of cationic polypeptides from one side of the membrane to the other. For example, when two electrostatic binding sites were introduced, at the entry and exit of the nanopore, both the rate constants of association and dissociation increased substantially, diminishing the free energy barrier for translocation.

[1]This work is funded by Syracuse University start-up funds and the US National Science Foundation, Grant DMR-706517

2:03PM J16.00011 Imaging Protein-Functionalized Quantum Dot Diffusion and Binding at Surfaces[1] , JACK RIFE, JAMES LONG, LLOYD WHITMAN, Naval Research Laboratory — Understanding single biomolecule and nanoparticle interactions with surfaces at fluid-solid interfaces is a key to improving molecular transport and binding in many biotechnology applications. Biosensor sensitivity, for example, is typically limited by diffusion [2] and non-specific binding to analytical surfaces. We have assembled a Total Internal Reflectance Fluorescence (TIRF) microscopy system with single-photon-sensitive cameras to image diffusion and binding of fluorescently-labeled biomolecules on surfaces under both static and laminar flow conditions. We have acquired movies (57 frames/s) of streptavidin-functionalized CdSe quantum dots (QDs) diffusing, transiently attaching, and permanently immobilizing on repulsive, hydrophilic silica surfaces. From the single-particle trajectories we have extracted diffusion coefficients and transient attachment lifetimes. The binding of protein-functionalized QDs to our nominally repulsive surfaces can be attributed to surface defects, adsorbates, and protein conformational changes. In flow, the QD elevation above the no-slip surface can be approximated, giving a picture of elevated transport between transient attachments and QD departures to and from the surface. [2] Sheehan and Whitman, Nano Lett. 5, 803 (2005).

[1]Supported by the DTRA, Joint Science and Technology Office

Tuesday, March 11, 2008 2:30PM - 5:30PM –

Session L3 DFD: The Physics of Climate and Climate Change Morial Convention Center RO2 - RO3

2:30PM L3.00001 The Disordered Kinetics of Earth's Carbon Cycle , DANIEL ROTHMAN, Department of Earth, Atmospheric, and Planetary Sciences, MIT — The carbon cycle describes the transformations of carbon as it cycles through living organisms and the physical environment. In its simplest form, the cycle amounts to a loop between photosynthesis and respiration. Photosynthesis produces organic carbon and molecular oxygen from carbon dioxide and water. Respiration reverses the process by oxidation of organic carbon. The duration of the cycle spans a vast range of time scales: from days or less for fast-growing plankton in the oceans, to hundreds of millions of years or more for the small fraction of organic matter that is buried as rock. The rates at which the cycle is closed set atmospheric carbon dioxide levels at short time scales and oxygen levels at geologic time scales. Respiration rates thereby influence not only climate—by the determination of equilibrium carbon dioxide concentrations—but also biological evolution—because the oxygenation of Earth's atmosphere must have preceded the advent of aerobic metabolism. We review recent advances in the understanding of the rates that control the carbon cycle, with emphasis on the respiratory back-reaction. Given considerable biological, chemical, and environmental variation, it comes as no surprise that measurements of rates vary greatly. Observations suggest, however, some surprising simplicity: for example, the rates of microbial consumption of organic matter in sediments and soils slow down systematically like the inverse of the age of the organic matter. This aging effect can be quantitatively understood as the macroscopic observation of microscopically disordered kinetics. The disorder can arise purely physically as the consequence of a reaction-diffusion process in porous media, but any combination of physical, chemical, and biological parameters that yield a wide range of rates suffices. A predicted practical consequence is a slow, logarithmic decay of organic matter in sediments and soils, which compares well with measurements. Further observations suggest that the effects of such disordered kinetics extends to inorganic processes as well. The carbon cycle thus appears not as a simple reaction network defined by a single set of rates, but rather as complex network in which the rates of specific reactions can be widely dispersed. We conclude by briefly discussing implications for short-term climate and long-term evolution.

3:06PM L3.00002 The Quantum and Fluid Mechanics of Global Warming[1] , BRAD MARSTON, Brown University — Quantum physics and fluid mechanics are the foundation of any understanding of the Earth's climate. In this talk I invoke three well-known aspects of quantum mechanics to explore what will happen as the concentrations of greenhouse gases such as carbon dioxide continue to increase. Fluid dynamical models of the Earth's atmosphere, demonstrated here in live simulations, yield further insight into past, present, and future climates. Statistics of geophysical flows can, however, be ascertained directly without recourse to numerical simulation, using concepts borrowed from nonequilibrium statistical mechanics[2]. I discuss several other ways that theoretical physics may be able to contribute to a deeper understanding of climate change[3].

[1]Supported in part by NSF grant no. DMR-0605619.

[2]J. B. Marston, E. Conover, and Tapio Schneider, "Statistics of an Unstable Barotropic Jet from a Cumulant Expansion," arXiv:0705.0011, J. Atmos. Sci. (in press).

[3]J. Carlson, J. Harte, G. Falkovich, J. B. Marston, and R. Pierrehumbert, "Physics of Climate Change" 2008 Program of the Kavli Institute for Theoretical Physics.

3:42PM L3.00003 Geostrophic Turbulence and the stability of Ocean models , ANNALISA BRACCO, Georgia Tech — Despite multiple efforts, predictions of climate change remain uncertain. Where precision is an issue (e.g., in a climate forecast), only ensembles of simulations made across model families which differ for parameterizations, discrete algorithms and parameter choices allow an estimate of the level of imprecision. Is this the best we can do? Or is it at least conceptually possible to reduce these uncertainties? Focusing on ocean models in idealized domains we describe chaotic space-time patterns and equilibrium distributions that mimic nature. Using the Navier-Stokes equations for barotropic flows as a zero-order approximation of analogous flow pattern, we then investigate if is possible, in this overly-simplified set-up, for which smooth-solutions exist, to bound the uncertainty associated with the numerical domain discretization (i.e. with the limitation imposed by the Reynolds number range we can explore). To do so we analyze a series of stationary barotropic turbulence simulations spanning a range of Reynolds number of 10^4.

4:18PM L3.00004 Heat waves, climate change and eggplant harvests - simple models of climate systems , ANTONELLO PROVENZALE, ISAC-CNR, Torino, Italy — I discuss a simple box model of soil-vegetation-atmosphere interactions that we recently introduced to study the insurgence of summer droughts at continental midlatitudes (D'Andrea et al, GRL 2006, Baudena et al, AWR 2007). I show that the model possesses multiple equilibria and that, for the same synoptic forcing, soil moisture at the beginning of summer and vegetation cover play a primary role in determining which equilibrium will be reached. We also observe a difference in the drought climatologies associated respectively with the dynamics of natural vegetation, capable of adapting to the prevailing soil moisture conditions, and with cultivated vegetation such as eggplant, that cannot spontaneously modify its areal extent. I conclude with some speculations on a conceptual model of the interaction between vegetation and climate at global scale. The results discussed in this talk are the product of joint work with Fabio D'Andrea (ENS, Paris) and Mara Baudena (ISAC-CNR).

4:54PM L3.00005 Physical Problems in Modeling the Global Ocean , STEPHEN GRIFFIES, NOAA/Geophysical Fluid Dynamics Lab — Understanding and modeling the physical ocean circulation is of primary importance for both enhancing the science of the ocean, and for providing rational projections of future climate. This talk aims to outline fundamental physical and numerical aspects of ocean climate modeling. We highlight features associated with representing elements of the continuum ocean fluid using a discrete model lattice. A major challenge of this representation includes the parameterization of scales which are unresolved by the simulation. This subgrid-scale problem is ubiquitous in computational fluid dynamics, and forms a major focus of ongoing research and development with ocean climate models. Another challenge involves developing robust numerical methods whose truncation errors do not adversely corrupt the quasi-ideal nature of much of the ocean circulation outside of boundary layers. Progress has been made on both fronts, with improvements arising from better understanding of the ocean, smarter methods used to simulate the ocean, and enhancements in computational power.

Tuesday, March 11, 2008 2:30PM - 5:30PM –

Session L9 DFD: Colloidal Self Assembly and Interactions Morial Convention Center RO7

2:30PM L9.00001 Tunable Liquid Micromirror Based on Self-Assembly of "Janus" Particles , TOM KRUPENKIN, University of Wisconsin - Madison, MIKE BUCARO, PAUL KOLODNER, Bell - Labs, Alcatel - Lucent, J. ASHLEY TAYLOR, University of Wisconsin - Madison — In optofluidics, control over light propagation is primarily achieved by using the optical properties of liquid-gas and liquid-liquid interfaces. Currently, the vast majority of existing optofluidic systems are refractive optical devices. However, reflective optofluidic devices potentially have a number of important advantages over their refractive counterparts, since they are not constrained by the relatively low refractive index contrast commonly found in liquid-liquid and liquid-gas interfaces. In this work, we propose and experimentally demonstrate a novel approach that makes it possible to create tunable reflective liquid surfaces by combining the flexibility and tunability of liquid-liquid interfaces with the excellent reflective properties of solid metal surfaces. We employ self-assembly of reflective solid "Janus" particles at the interfaces between polar and non-polar liquids to create highly flexible, continuous, reflective "carpets" capable of acting as spherical micromirrors. We have successfully demonstrated electrowetting-based dynamic tuning of these micromirrors, including electrical control over mirror shape and focal distance. The mirror self-assembly process was studied as a function of the particle functionalization and of the chemical properties of the liquids involved. Potential applications of the proposed mirrors are also discussed.

2:42PM L9.00002 Emerging Structures for Colloidal Brushes: from Dispersions and Agglomerates to Spherulites, Wires, and beyond , ALBERTO STRIOLO, University of Oklahoma — A large variety of nanoparticles holds extraordinary promises for practical applications, e.g., in catalysis and materials science. For these and other applications it is necessary to assemble the nanoparticles to yield supra-molecular aggregates of desired morphology. We are interested in the self-assembly of spherical colloids (i.e., nanoparticles) induced by interactions that become anisotropic because of entropic effects. Thus short polymer brushes are grafted on restricted regions of the spherical nanoparticles considered (e.g., the equatorial plane). Monte Carlo simulations were conducted to assess the properties of the self-assembled nanostructures as a function of the length of the brushes and of the strength of the particle-particle attraction. Depending on the specific solution conditions (particle-particle dispersive attractions, as well as length and density of the grafted polymer brushes) it is possible to obtain uniform dispersions, irregular aggregates, spherulites, one-dimensional wires, and two-dimensional colloidal sheets. We will discuss whether or not the effective colloid-colloid pair interactions at infinite-dilute conditions (i.e., the potential of mean force) can be used to predict the emerging behavior of the colloidal nanoparticles at larger concentrations.

2:54PM L9.00003 Roughness-controlled depletion interactions for controlling colloidal self-assembly , KUN ZHAO, Dept. of Chemistry, University of California- Los Angeles, THOMAS G. MASON, Depts. of Physics and Chemistry, University of California- Los Angeles — The surfaces of colloidal particles resulting from many new fabrication methods are not molecularly smooth, so understanding how the surface roughness affects the depletion attraction is very important. We show that the depletion attraction between custom-shaped microscale platelets can be suppressed when the nanoscale surface asperity heights become larger than the depletion agent. In the opposite limit, the attraction re-appears and columnar stacks of platelets are formed. Exploiting this, we selectively increase the site-specific roughness on only one side of the platelets to direct the mass-production of a single desired assembly: a pure dimer phase. Furthermore, we model the interaction between flat plates coated by hemispheres having controlled sizes and densities relative to those of a spherical depletion agent. Overall, these studies provide significant insight into attractive bonds between particles that retain lubrication, and they provide a basis through which more complex assemblies can be made.

3:06PM L9.00004 Corralled Colloids in Four Dimensions , STEPHEN ANTHONY, Department of Chemistry, University of Illinois, MINSU KIM, Department of Physics, University of Illinois, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois — Three colloidal particles were placed in small corrals and the strong correlations between their translation and rotation were quantified using the optical anisotropy of MOON (Modulated Optical Nanoprobes) particles to simultaneously measure their translation and rotation in an optical microscope. This system represents the simplest system which can capture one of the relevant components of multi-body interactions, the fact that while two particles can freely rotate together (like gears), once a third particle (or gear) is added there is no universally favorable set of rotations. This simple multi-body system provides a paradigm of how rotation influences translation and vice-versa.

3:18PM L9.00005 Interactions among microdroplets at the water-air interface , CHUAN ZENG, Department of Physics, University of Massachusetts Amherst, ANTHONY D. DINSMORE — There has been a great mystery concerning the origin of measured long-range attraction among microparticles at fluid interfaces. Recent theoretical work[1] showed that electrostatic interactions should not lead to long-range attraction, but the possibility remains that attraction arises from an irregular contact line on the particles' surfaces. Replacing the solid particles with liquid droplets eliminated surface roughness and thus reduced the complexity of the system. We captured micron-sized oil droplets at water-air interface and measured the interaction between them. The dynamics of droplets at interface were imaged using optical microscopy, from which the droplets' motions were tracked and analyzed. The interaction between two isolated droplets was calculated from their trajectories through the Markovian dynamics extrapolation method developed by J. C. Crocker and D. G. Grier[2]. We acknowledge support from NASA through the Fluid Physics program (NRA 02-OBPR-03-C) and from the NSF-supported MRSEC on Polymers (DME-0213695).

[1] See, for example, M. Oettel, A. Dominguez, and S. Dietrich, *Phys. Rev. E* **71**, 051401 (2005).
[2] J. C. Crocker and D. G. Grier, *Phys. Rev. Lett.* **73**, 352 (1994).

3:30PM L9.00006 Geometrical frustration in colloidal "antiferromanget"[1] , YILONG HAN, Hong Kong University of Science and Technology, YAIR SHOKEF, AHMED ALSAYED, PETER YUNKER, TOM LUBENSKY, ARJUN YODH, University of Pennsylvania — We report experiments about a self-organized colloidal system that exhibits geometrical frustration similar to that of antiferromagnetic Ising spins on a triangular lattice. Novel thermally sensitive microgel NIPA (N-isopropyl acrylamide) spheres are close packed between two parallel flat walls with a vertical separation of about 1.5-particle diameters. The particles form an approximate in-plane triangular lattice. Neighboring particles tend to push each other toward opposite walls leading to out-of-plane local up and down buckling. We tune the strength of such effective antiferromagnetic interactions by varying temperature-tunable diameter of spheres. "Spin" flipping was directly visualized with video microscopy. We investigated the static structures, the dynamics of particles with different degrees of frustration and the degenerated ground state. This experiment is the first dynamic measurement in a geometrical frustrated system at single-particle resolution.

[1]This work is supported by the MRSEC grant DMR-0520020 and NSF grant DMR-0505048.

3:42PM L9.00007 Correlated Motion of Ellipsoids Diffusing in 3D , KENNETH DESMOND, ERIC R. WEEKS, Emory University — Currently the hydrodynamic interaction between two ellipsoids in a fluid is not well understood. By observing the Brownian motion of micron sized ellipsoids suspended in a fluid using confocal microscopy, we directly measure these interactions. The ellipsoids exhibit both translational and rotational diffusion. The motion of an ellipsoid induces a flow field, which couples the motion of other ellipsoids with the first one. In our experiments we measure the translational and rotational diffusion of polystyrene ellipsoids suspended in a water glycerol mixture in three dimensions, and examine the spatial correlations between the rotational and translational motion of pairs of ellipsoids. Rotational motions set up a dipolar flow field, and thus the resulting correlations decay quicker than the correlations caused by translations.

3:54PM L9.00008 Simulating Collective Dynamics of Confined Colloids[1] , JONATHAN K. WHITMER, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — We investigate the dynamical behavior of colloidal particles under confinement, by means of computer simulations that explicitly account for hydrodynamic interactions. Even under dilute conditions, long-range solvent-mediated coupling of the translational and rotational degrees of freedom influences the relative motion of colloidal particles. These effects on the collective dynamics are often ignored in simulations. Our calculations utilize the hybrid Stochastic Rotation Dynamics/Molecular Dynamics method [A. Malevanets and R. Kapral, J. Chem. Phys. **112**, 7260 (2000)] to incorporate both hydrodynamic and Brownian forces exerted on colloids by the solvent. The computational results are compared to recent experiments on few-body colloidal systems where the particle number is limited through confinement in a cylindrical trap.

[1]This work is supported by the National Science Foundation through Grant No. DMR-0346914.

4:06PM L9.00009 Stripes and their zigzagging in buckled hard spheres , YAIR SHOKEF, University of Pennsylvania, YILONG HAN, Hong Kong University of Science and Technology, AHMED ALSAYED, PETER YUNKER, TOM LUBENSKY, ARJUN YODH, University of Pennsylvania — We use a hard sphere model to describe recent experiments on buckled colloidal monolayers. Our detailed Monte Carlo simulations exhibit the behavior, observed experimentally, of antiferromagnetic order and the formation of stripes that randomly zigzag around the system. Using free volume calculations, we deduce the strength of the effective antiferromagnetic interactions between neighboring particles. We furthermore explain how the geometrical frustration is partially removed by collective effects arising from sphere packing. We show how lattice distortions enable striped configurations to pack better than disordered ground states of the simple antiferromagnetic Ising model and that zigzagging of these stripes does not affect the free volume of the system.

4:18PM L9.00010 Breakdown of Pairwise Additivity in Colloidal Electrostatics[1] , SUNIL SAINIS, Yale University, Mechanical Engineering Department , ERIC DUFRESNE, Yale University, Departments of Mechanical Engineering, Chemical Engineering and Physics — Predictions of the structure and stability of charged colloidal suspensions typically assume pairwise additive forces. We directly measure electrostatic forces in small clusters of two to seven particles in a nonpolar solvent. We find that electrostatic interactions are not pairwise additive when the particle separations are much smaller than the screening length.

[1]Yale University, Sandia NINE, Cabot Corp.

4:30PM L9.00011 Mystery on Charge Asymmetry: Anionic Macroions in Periodic Lattices Held by Hydrated Cations and Not vice versa[1] , WILLIAM KUNG, MONICA OLVERA DE LA CRUZ, Northwestern University — We propose a mean-field analytical model to account for the observed asymmetry in the ability to form long-range attraction by the negatively charged colloidal particles and not their equivalently charged positive counterpart. We conjecture that this asymmetry is due to solvation effects, and we phenomenologically capture its physics by considering the relative strength of this water-induced short-range repulsion between the different charge species. We then apply our model to the colloidal system of negatively charged disks that are neutralized by a sea of counterions and strongly absorbed to an interface in a compressible binary system. We demonstrate the resulting coexistence between a dilute isotropic ionic phase and a condensed hexagonal lattice phase as a function of density and interaction strength.

[1]ACS-PCF Grant 44645-AC7.

4:42PM L9.00012 Charged colloids in low polar solvents , ANDREW HOLLINGSWORTH, MIRJAM LEUNISSEN, WILLIAM IRVINE, PAUL CHAIKIN, New York University, ALFONS VAN BLAADEREN, Utrecht University — In a low polar environment, sterically-stabilized poly(methyl methacrylate) spheres become positively charged and exhibit extraordinary long-range repulsive interactions. Confocal microscopy shows that they can form low density, body centered cubic crystals with lattice constants up to 40 microns. We attribute this behavior to the cyclohexyl bromide (CHB) in which the colloidal particles are suspended. CHB is a desirable solvent due to its density matching capability; however, it is difficult to purify. Trace amounts of the hydrogen halide resulting from the hydrolysis of CHB apparently interact with the stabilizer layer, imparting charge to the colloids. Surprisingly, water can also be used to deionize the organic solvent, depending on the relative amounts of the two fluids. The addition of quaternary ammonium salts was used to screen charge (reducing long range particle interaction). Ionic strengths were computed using ionic association theory; in turn, particle charge and surface potentials were estimated from electrokinetic measurements.

4:54PM L9.00013 Direct measurements of the pair potentials of colloids with light scattering and optical traps , KISUN YOON, SEAS, Harvard University, VINOTHAN MANOHARAN, Department of Physics, SEAS, Harvard University — We present a methodology of directly measuring the pair potentials of colloids. We take snapshots of the thermal fluctuation of a pair of colloidal particles in equilibrium. The probability distribution of the separation distance obtained from the snapshots should follow the Boltzmann distribution because the separation distance of the particle pair is the only independent variable necessary to describe the effective free energy of a macrostate of the colloidal particle pair in equilibrium. The measurement of the pair potentials can be achieved by appropriately subtracting the unwanted potentials due to optical traps and optically induced interactions from the effective free energy. Accurate measurement of the separation distance between colloidal particles has critical importance in measuring colloidal interactions. Conventional Video Microscopy used for separation distance measurement is significantly restricted due to the two-dimensional nature of the measurement. Furthermore, the measurement is seriously distorted when the two particles are nearly in contact because of the diffraction of light and multiple scattering effect. We introduce a new technique to accurately measure the separation distances using light scattering. This light scattering technique can measure the separation distance in 3D and appropriately considers the multiple scattering effect.

5:06PM L9.00014 Concentration Gradients in Mixed Magnetic and Nonmagnetic Colloidal Suspensions , RANDALL ERB, BENJAMIN YELLEN, Duke University — The ability to form concentration gradients in mixed magnetic/nonmagnetic colloidal suspensions using magnetic field gradients has many practical applications in the fields of biosensors and life science diagnostics. Previously, we developed and experimentally confirmed a self-consistent model describing the local distribution of magnetic nanoparticles exposed to a magnetic field gradient. Here, we have derived an analytic expression to describe the local concentration of nonmagnetic colloids which are also affected by field gradients when inside magnetic colloidal suspensions. The model calculates the force on particles as a function of local magnetic particle concentration, and solves for the equilibrium distribution of particles through the drift-diffusion equations. We investigate the ability to concentrate and deplete nonmagnetic particles from specific regions of a substrate, such as nearby patterned micro-magnets on a substrate. Also, we have qualitative experimental results to support our expression. Our results show that nonmagnetic particles which are 5-10 times larger than the magnetic nanoparticles can be effectively concentrated or depleted at specified regions of the substrate.

5:18PM L9.00015 Interactions and self assembly of two heterogeneously charged surfaces , ROBERT BREWSTER, Dept. of Materials And Interfaces, Weizmann Institute of Science, PHILIP PINCUS, Dept. of Physics, SAMUEL SAFRAN, Dept. of Materials And Interfaces, Weizmann Institute of Science — Recent experiments[1,2] have measured attractive interactions between two surfaces that each bear two molecular species with opposite charge. Theoretical considerations predict equilibrium finite-sized domains of each species, consistent with experiment. These domains, whose observed sizes are typically tens of nanometers, are the result of a balance between the line tension, which prefers macroscopic separation, and the electrostatics, which prefers mixing. Additionally, two such surfaces show a long range attraction. We present a theoretical model that predicts the domain size, phase behavior and forces for two such interacting surfaces.

(1) E. E. Meyer, Q. Lin, T. Hassenkam, E. Oroudjev, J. N. Israelachvili PNAS **102**, 6839 (2005).
(2) S. Perkin, N. Kampf, J. Klein, Phys. Rev. Lett. **96**, 038301 (2006).

Wednesday, March 12, 2008 8:00AM - 11:00AM –

Session P6 DFD: Fluid Dynamics and Biology Morial Convention Center RO4

8:00AM P6.00001 Depolymerization-driven flow and the crawling of nematode sperm , CHARLES WOLGEMUTH, UCONN Health Center — Cell crawling motility is integral in many biological and biomedical processes, such as wound healing, cancer metastasis, and morphogenesis. A complete understanding of the mechanisms by which cells crawl is still lacking, but it is known to entail at least three separate physical processes: (i) cytoskeletal extension at the front of the cell; (ii) adhesion to the substrate at the cell front and release at the rear; and (iii) advance of the cell body. In most cells, the cytoskeletal network is composed of actin. The mechanism by which force is generated to drive translocation of the cell body is still debated. Originally, this force was attributed to an actomyosin system similar to muscle. However, nematode sperm utilize a cytoskeleton composed of a network of Major Sperm Protein (MSP) that forms non-polar filaments for which molecular motors have not been identified. The motility of these cells still exhibits all three fundamental processes required for standard crawling motility. Experiments suggest that depolymerization of the cytoskeletal network is the force-producing mechanism for pulling up the rear. In this talk I will present a mechanical model that describes how depolymerization of the cytoskeleton can drive motility. This model accounts for both cytoskeletal displacements and cytsolic (the fluid component of the cell) flow. The model accurately fits in vitro data using nematode sperm extracts where depolymerization induces contraction of MSP polymer bundles. Application of this model to cell crawling produces testable predictions about how the size and shape of a cell affect crawling speed. Experiments using *Caenorhabditis elegans* sperm show good agreement with the model predictions. Interestingly, the model requires that cells are anisotropically elastic, being more stiff in the direction of motion than perpendicular to it. A simple physical picture can account for this anisotropy. The model also predicts that cell speed increases with anisotropy and with depolymerization rate.

8:36AM P6.00002 Optimizing Low Reynolds Number Locomotion , ANETTE HOSOI, MIT — In this talk I will discuss optimal stroke patterns for low Reynolds number linked swimmers. We begin by optimizing stroke patterns for Purcell's 3-link swimmer modeled as a jointed chain of three slender links moving in an inertialess flow. The swimmer is optimized for efficiency and speed and we are able to attain significant increases is efficiency over those previously suggested by authors who only consider geometric design rather than kinematic criteria. We then go on to investigate uniflagellate and biflagellate organisms and compare the optimized results to biological data from spermatozoa and chlamydomonas.

9:12AM P6.00003 Instabilities and pattern formation in active particle suspensions[1] , DAVID SAINTILLAN, Courant Institute, New York University — Suspensions of swimming microorganisms are characterized by complex dynamics involving strong fluctuations and large-scale correlated motions. These motions, which result from the many-body interactions between particles, are biologically relevant as they impact mean particle transport, mixing and diffusion, with possible consequences for nutrient uptake. Using direct numerical simulations, I first investigate aspects of the dynamics and microstructure in suspensions of interacting self-propelled rods at low Reynolds number. A detailed model is developed that accounts for hydrodynamic interactions based on slender-body theory. It is first shown that aligned suspensions of swimming particles are unstable as a result of hydrodynamic fluctuations. In spite of this instability, a local nematic order persists in the suspensions over short length scales and has a significant impact on the mean swimming speed. Consequences of the large-scale orientational disorder for particle dispersion are discussed and explained in the context of generalized Taylor dispersion theory. Dynamics in thin liquid films are also presented, and are characterized by a strong particle migration towards the interfaces. The results from direct numerical simulations are then complemented by a kinetic model, in which the dynamics are captured using a continuity equation for the particle configurations, coupled to a mean-field description of the flow arising from the active stress exerted by the particles on the fluid. Based on this model, the linear stability of both aligned and isotropic suspensions is revisited. In aligned suspensions, the instability observed in the simulations is predicted to occur at all wavelengths, a result that generalizes previous predictions by Ramaswamy et al. (2002). In isotropic suspensions, an instability for the active particle stress is also found to exist, in which shear stresses are eigenmodes and grow exponentially at long scales. Non-linear effects are also investigated using numerical simulations in two-dimensions. The results of the stability analysis are confirmed, and the long-time non-linear behavior is shown to be characterized by strong density fluctuations, which appear to be driven by the active stress instability.

[1]This work is in collaboration with Michael Shelley (NYU)

9:48AM P6.00004 Life in a drop of Ocean: microfluidic insights into microbial ecology , ROMAN STOCKER, Civil and Environmental Engineering - MIT — Bacteria are the most abundant and successful form of life on Earth. Their physico-chemical interactions with their fluid environment are surprisingly complex and have enormous implications, which we can only hope to grasp if we learn to study microorganisms within realistic microenvironments. Microfluidics for the first time enables us to create microhabitats, including chemical and fluid mechanical landscapes, while visualizing bacterial behavior at a single-cell resolution. Here I focus on the application of microfluidics to gain insight in the life of marine bacteria. In their quest for nturients, marine bacteria often experience the Ocean as a desert, where rare and ephemeral nutrient patches represent transient resource oases. In this patchy seascape, swimming and chemotaxis represent critical assets, but effective patch utilization is constrained by energetic requirements. And then there are predators and viruses... These interactions form the basis of the 'microbial loop', the ensemble of microbial processes known to directly impact the productivity of marine ecosystems and the rates of carbon turnover in the Ocean. I will show how fundamental new insight on selected aspects of microbial life in a drop of Ocean can be achieved by a combination of microfluidic experiments and theoretical modeling.

10:24AM P6.00005 Optimal flexibility in flapping appendages[1] , SILAS ALBEN, Georgia Institute of Technology — When oscillated in a fluid, appendages such as insect wings and fish fins can produce large thrust forces while undergoing considerable bending. Can we understand these bending patterns by comparing them with the patterns which produce maximum thrust, or a given thrust at maximum efficiency? We present a general model for how flexible surfaces produce vorticity and bend actively and passively in a fluid. We solve the model numerically, and discuss results for moderate deflections (relevant for large thrust), and for small deflections (relevant for high efficiency). We'll then consider how a fish-fin-like structure might be designed for optimal performance.

[1]We acknowledge support from the NSF Division of Mathematical Sciences

Wednesday, March 12, 2008 8:00AM - 11:00AM –
Session P8 DFD: Glassy Dynamics Morial Convention Center RO6

8:00AM P8.00001 Nonlinear Dynamics Near the Jamming Transition , EDWARD J BANIGAN, Dept of Physics and Astronomy; Univ of Pennsylvania, DAVID A EGOLF, Department of Physics, Georgetown University — How dynamical behaviors and static measures are related near the jamming transition remains an open question. In simulations of a two-dimensional sheared granular cell, we have calculated mathematical quantities that characterize the underlying nonlinear dynamics near the jamming transition. We find that the Lyapunov exponents and vectors characterizing the most important dynamical modes correlate well in space and time to localized events that alter the physical characteristics of the system. For example, the Lyapunov exponents and vectors highlight areas in which particles are involved in cooperative rearrangement or the formation or destruction of stress chains. In at least some cases, the behavior of the dynamical quantities appears to indicate future position or stress rearrangements. In addition, we report measurements of a dynamical time scale and a dynamical length scale that diverge as the system jams, suggesting an intriguing connection between the jamming transition and a transition between chaotic and non-chaotic dynamical states.

8:12AM P8.00002 Probing Cooperative Motion in Super-Cooled Colloidal Suspensions , PRASAD SARANGAPANI, Y. ELAINE ZHU, University of Notre Dame, Department of Chemical and Biomolecular Engineering, 182 Fitzpatrick Hall, Notre Dame, IN 46556 — The physics of the glass transition remains inadequately understood despite its broad technological relevance. The anomalous divergence of viscosity without apparent structural change as a liquid is cooled has been attributed to the existence of growing dynamic length scales of "cooperatively rearranging regions" (CRR). In this work, we use ultra-fast fluorescence correlation spectroscopy (FCS) combined with high-speed imaging to determine the CRR sizes by measuring single-particle dynamics of tracer nano-particle embedded in super-cooled "hard-sphere" colloidal suspensions. Fluorescent poly-(methyl methacrylate) (PMMA) tracer particles of radii ranging from r =0.1-0.4 μm, mixed with plain PMMA particles of radius, r =0.6 μm and bulk volume fraction, ϕ = 0.38-0.58, serve as excellent probes for changes in the energy barrier landscape of the suspensions of increasing volume fraction and are sensitive to the creation and annihilation of icosahedral order in metastable colloidal fluids. We also find that the correlation length, determined by fluctuation-dissipation relations from the measured auto-correlation functions, shows a dramatic increase in the super-cooled regime until it diverges at ϕ=0.58.

8:24AM P8.00003 Structural relaxation in sheared two-dimensional foams , MATTHIAS MOBIUS, GIJS KATGERT, MARTIN VAN HECKE, University of Leiden — Athermal and disordered systems at rest, such as foams and granular media, are stuck in a meta-stable configuration. Upon shear the system unjams and complex vortex-like rearrangements ensue that are correlated in time and space. In our experiment we investigate what the typical time scales of these structural relaxations are as a function of the local shear rate in a two-dimensional, disordered foam that is linearly sheared. After an initial super-diffusive regime, the bubbles become diffusive at later times. This transition is reflected in the statistics of the bubble displacements, which are initially strongly correlated and non-Gaussian but eventually become Gaussian. We find that the relaxation time decreases with shear rate. For large shear rates the dependence follows a power law with an exponent significantly different from -1.

8:36AM P8.00004 From spontaneous to induced dynamic fluctuations: Granular packings as an experimental probe , FREDERIC LECHENAULT, North Carolina State University, OLIVIER DAUCHOT, SPEC, CEA France, GIULIO BIROLI, SPhT, CEA France, JEAN-PHILIPPE BOUCHAUD, Science & Finance, Capital Fund Management — We track the motion of a horizontally vibrated amorphous assembly of bidisperse hard disks, for densities ranging across the jamming transition. The spatial extension of dynamical heterogeneities and the associated relaxation time are found to exhibit critical behavior. Moreover, a dynamical fluctuation inequality relating the dynamical susceptibility χ_4 and the response of the dynamics to a change in density is tested. As the diffusion length is found to rescale these quantities, the dependencies of the inequality on length and time scales as well as density can be evaluated independently. Surprisingly, the lower bound is found to reproduce the non-monotonic behavior of χ_4 in time, which reveals an intimate link between dynamical heterogeneity and marginal super diffusion. Finally, the bound is shown to be tight and to mimic the anomalous features of the dynamical susceptibility across the transition.

8:48AM P8.00005 Influence of the microstructure on jammed packings of spheres , ERIC CORWIN, MAXIME CLUSEL, ALEXANDER SIEMENS, JASNA BRUJIC, New York University — Jammed matter is by definition impenetrable to light, such that little is known about the geometry of jammed systems. Using confocal microscopy to image an emulsion in 3D, we use the enhanced fluorescence at the droplet contacts to determine the contact network inside this model frictionless system. This enables the experimental determination of the average coordination number $< Z >$, which agrees with the isostatic predicted value of $< Z > \simeq 6$ [1]. Furthermore, we measure the distribution of coordination numbers within the jammed packings close to the isostatic limit. We show that the distribution of sizes of the droplets strongly influences the coordination number distribution, as well as the volume fraction at which the system becomes jammed. This may have important consequences on the stress propagation properties of the material as a whole. [1] J. Brujić *et al.*, Phys. Rev. Lett. 98, 248001 (2007)

9:00AM P8.00006 Mode-coupling and generalized mode-coupling theory: a diagrammatic approach , GRZEGORZ SZAMEL, Department of Chemistry, Colorado State University — We present a diagrammatic approach to the dynamics of interacting Brownian particles. Within this approach, the time-dependent density correlation function is represented by a series of diagrams with three and four leg vertices. We analyze the structure of this series and obtain a diagrammatic interpretation of reducible and irreducible memory functions. The one-loop self-consistent approximation for the latter function coincides with mode-coupling approximation for Brownian systems that was derived previously using a projection operator approach. Finally, we investigate the diagrammatic interpretation of a generalized mode-coupling theory.

9:12AM P8.00007 Percolating Clusters in Systems of Gapped Rigid Rings.[1] , CHRISTOPHER LASOTA, ARIEL HELFER, Kenyon College — We have examined the behavior of kinetically agitated collections of rigid rings with angular gaps in them. For small gap angles, large clusters form readily and are sufficiently tangled so that they may be raised vertically under gravitational stresses without decomposing. Using gravity as a stressor under semi-static conditions, we have measured average cluster size as a function of the gap angle and witness what appears to be a second order percolation phase transition. The critical gap angle depends somewhat on the relative thickness of the ring material compared to the ring diameter. Although friction is necessary for the formation of clusters, it appears that cluster formation is dominated by geometry effects.

[1]This work supported by Kenyon College

9:24AM P8.00008 Jamming transition in a temperature-sensitive 2D colloidal suspension[1] , ZEXIN ZHANG, DANIEL T. N. CHEN, ARJUN G. YODH, University of Pennsylvania, KEVIN B. APTOWICZ, West Chester University, PIOTR HABDAS, Saint Josephs University — We experimentally investigate the jamming transition of a 2D colloidal system. The system consists of a bidisperse mixture of thermoresponsive microgel particles confined between two glass slides, with a thickness of roughly the diameter of the larger particle. The packing density of the system is tuned by changing the temperature. A range of packing densities, both below and above the jamming transition is studied. We use video microscopy and particle tracking techniques to characterize the motion of the particles. On approaching the jamming transition the motion becomes slower and more heterogeneous. We characterize the jamming transition in terms of both structure (pair correlation function) and dynamics (mean square displacement, non-Gaussian parameter, four-point susceptibility). To our knowledge this study provides the first experimental evidence for the jamming transition in a 2D colloidal system.

[1]This work was support by MRSEC grant DMR-0520020 and NSF grant DMR-0505048

9:36AM P8.00009 Exact Enumeration of Jammed States for Confined Hard Discs[1] , S.S. ASHWIN, Department of Chemistry, Universiy of Saskatchewan, RICHARD K. BOWLES, Department of Chemistry, University of Saskatchewan — Enumeration of jammed states of particle systems interacting with hard potentials such as hard discs and hard spheres is a long- standing problem which holds the key to understanding the nature of glassy dynamics and the question of the possibility of an ideal glass transition in these systems. A simple model consisting of hard discs (of diameter σ) trapped between two hard lines separated by a distance H exhibits slow relaxation and heterogeneous dynamics characteristic of glassy systems. We map the locally jammed structures in this model to tiles and pose the problem of enumeration of jammed states for the case $H < 2\sigma$, as a tiling problem on a subset of a plane. Further on applying constraints for collective jamming on the arrangement of the tiles, we exactly enumerate the entire jamming landscape of the system and explore how this landscape is connected to the thermodynamics and dynamics of the glassy system.

[1]We would like to thank NSERC and CFI for funding.

9:48AM P8.00010 Heterogeneities in granular dynamics , ANITA MEHTA, S N Bose National Centre for Basic Sciences, Calcutta, India — The absence of Brownian motion in granular media is a source of much complexity; among these is the presence of heterogeneity, whether static or dynamic, within a given system. Such strong heterogeneities can exist as a function of depth in a box of grains; this is the system we study here. We present results from three-dimensional, cooperative and stochastic Monte Carlo shaking simulations of spheres on heterogeneous density fluctuations. These are justaposed with results obtained from a theoretical model of a column of grains under gravity; frustrations via competing local fields is included in our model, while the effect of gravity is to slow down the dynamics of successively deeper layers. The combined conclusions suggest that the dynamics of a real granular column can be divided into different phases – *ballistic, logarithmic, activated* and *glassy* – as a function of depth. The nature of the ground states and their retrieval, in the glassy phase, shows clear evidence of *intrinsic* states, which lie below a band of approximately degenerate ground states. In the other three phases, by contrast, the system jams into a state chosen randomly from this upper band of metastable states.

10:00AM P8.00011 Confocal Microscopy of Shear-Induced Dynamics in Jammed Emulsions[1] , JOAQUIM CLARA-RAHOLA, ERIC R. WEEKS, Emory University - Physics Department — Emulsions are liquid droplets suspended in a second continuous fluid. We study polydisperse decane-in-water emulsions at droplet volume fractions of about 0.8. At such concentrations emulsions are jammed and the system exhibits the properties of a solid. Droplet rearrangements due to Brownian motion are limited in this jammed material. Thus, to induce droplet displacements at length scales above a particle diameter, an oscillatory strain is applied. We use confocal microscopy to track the trajectories of the droplets in real time and space. By taking advantage of this technique we quantify the affine and non-affine motion of the droplets due to the shear. Moreover, we study elastic and plastic droplet reconfigurations as well as the spatial extent of the rearrangements when the droplet volume fraction and polydispersity are varied.

[1]Swiss National Foundation

10:12AM P8.00012 Vacancy diffusion in a triangular lattice model , M. JENG, M. BOWICK, Syracuse University, W. KRAUTH, Laboratoire de Physique Statistique, Ecole Normale Superieure, J. M. SCHWARZ, X. XING, Syracuse University — We study vacancy diffusion in the classical triangular lattice dimer model, subject to the kinetic constraint that dimers can only translate, but not rotate. A single vacancy—i.e. a monomer—in an otherwise fully packed lattice, is always localized in a tree-like structure. The distribution of tree sizes is asymptotically exponential and has an average of 8.16 ± 0.01. A connected pair of monomers has a finite probability of being delocalized. When delocalized, the diffusion is anomalous: $\langle \vec{r}^2 \rangle \propto t^\beta$, with $\beta = 0.46 \pm 0.05$. The same diffusion law is also exhibited by clusters of three or four monomers. It is found that both swap motions (translations of dimers transverse to their axes) and glide motions (translations of dimers parallel to their axes) are essential for the large-scale diffusion of monomers.

10:24AM P8.00013 Studying microscopic rearrangements in a sheared supercooled colloidal liquid , DANDAN CHEN, DENIS SEMWOGERERE, JOAQUIM CLARA-RAHOLA, ERIC R. WEEKS, Emory University — Shearing induces complex microstructure changes inside an amorphous material, which is related to interesting phenomena like shear thicking and shear thinning. We use a colloidal suspension to simulate amorphous materials, and we study how shearing changes this structure using fast confocal microscopy. Many experiments and simulations have found macro-stress flucatuations in sheared dense jammed suspensions. However, the micro-rearrangements of the particles while being sheared are not very clear. We study the non-affine motion of the colloids, finding the particles move in groups, and characterize these groups for different shearing rates.

10:36AM P8.00014 Temperature control of attractive interactions in colloids , PETER SCHALL, University of Amsterdam, ZHIBING HU, University of North Texas — Attractive colloidal systems have attracted increasing interest recently: They exhibit phase behavior with solid, liquid, and gas phases, and various metastable states, ranging from gel-like to glassy. These colloidal systems offer a convenient way to investigate important phenomena such as phase formation and kinetic arrest. The most prominent colloidal systems are colloid-polymer mixtures, in which the attractive strength is fixed by the concentration of the added polymer. We present a colloidal system that allows variation of the attractive potential with external control: a binary liquid solvent gives rise to temperature-dependant particle attractions close to the demixing temperature of the liquid mixture. This allows us to use temperature control to induce transitions from gas to liquid to solid, or to form metastable gel-like or glassy states. Variation of the heating rate allows us to investigate the kinetics of these transitions. In this talk, I will focus on a novel system, in which close index- and density matching of the solvent and the particles is possible; this enables us to study bulk processes with temperature control.

10:48AM P8.00015 A thermodynamic equation of jamming , KEVIN LU, H. PIROUZ KAVEHPOUR, Department of Mechanical and Aerospace Engineering, UCLA — Materials ranging from sand to fire-retardant to toothpaste are considered fragile, able to exhibit both solid and fluid-like properties across the jamming transition. Guided by granular flow experiments, our equation of jammed states is path-dependent, definable at different athermal equilibrium states. The non-equilibrium thermodynamics based on a structural temperature incorporate physical ageing to address the non-exponential, non-Arrhenious relaxation of granular flows. In short, jamming is simply viewed as a thermodynamic transition that occurs to preserve a positive configurational entropy above absolute zero. Without any free parameters, the proposed equation-of-state governs the mechanism of shear-banding and the associated features of shear-softening and thickness-invariance.

Wednesday, March 12, 2008 8:00AM - 10:48AM –

Session P9 DFD: Microfluidic and Nanofluidic Devices Morial Convention Center RO7

8:00AM P9.00001 Microfluidic Fabrication of Bio-compatible Vesicles by Self-assembly in Double Emulsions , HO CHEUNG SHUM, Harvard School of Engineering and Applied Sciences, Harvard University, JINWOONG KIM, Amore Pacific Co. R&D Center, DAEYEON LEE, Harvard School of Engineering and Applied Sciences, Harvard University, DAVID WEITZ, Harvard School of Engineering and Applied Sciences, and Department of Physics, Harvard University — Vesicles are compartments surrounded by bilayered membranes of amphiphilic molecules such as diblock copolymers and phospholipids. To minimize the exposure of their hydrophobic part to water, amphiphilic molecules self-assemble into aggregates of different structures. When the hydrophobic to hydrophilic ratio is close to unity, amphiphiles self assemble into bilayers, which tend to fold themselves into vesicles. These vesicles are useful for encapsulating and transporting actives such as drugs, flavor, and fragrance. To solve the problems of low encapsulation efficiency and large vesicle size distributions afforded by traditional techniques to create vesicles, we engineer a novel route to generate vesicles using monodisperse double emulsions prepared in microfluidics as templates. The double emulsion-to-vesicle transition exhibits different behaviors depending on the properties of the amphiphilic molecules such as the hydrophobic-to-hydrophilic ratio. Using this technique, we have fabricated both bio-compatible diblock copolymer vesicles, also known as polymersomes, and also lipid vesicles with high encapsulation efficiency.

8:12AM P9.00002 Glass Coating for PDMS Microfluidic Channels by Sol-Gel Methods , THAO DO, ADAM ABATE, DAVID WEITZ, Harvard University — Soft lithography in polydimethylsiloxane (PDMS) allows one to fabricate complex microfluidic devices easily and at low cost. However, PDMS swells in the presence of many organic solvents, which can significantly degrade the performance of PDMS microfluidic devices. We present a method to coat PDMS channels with a glass-like layer using sol-gel chemistry. As a demonstration of chemical resistance, we flow toluene and aqueous Rhodamine B through coated PDMS channels. Toluene is an organic solvent that significantly swells PDMS in a matter of seconds. Rhodamine B is an organic fluorescent molecule that leaches into PDMS and can therefore be used as a fluorescent probe. Indeed, the coating suppresses swelling of the channels when exposed to toluene; it also prevents leaching of Rhodamine B into PDMS channels. In addition, the channels can be functionalized with silanes to precisely control surface properties. We exploit the high chemical resistance and precise surface functionalization of the coating to produce both direct toluene-in-water and inverted water-in-toluene emulsions in coated, functionalized, PDMS microfluidic channels. This combines the ease of fabrication afforded by soft-lithography with the precision control afforded by sol-gel glass.

8:24AM P9.00003 Fluid Flow and Heat Transfer in a Dual-wet Micro Heat Pipe , JIN ZHANG, STEPHEN WATSON, HARRIS WONG, Louisiana State University — Micro heat pipes have been used to cool micro electronic devices, but their heat transfer coefficients are low compared with those of conventional heat pipes. In this talk, a dual-wet pipe is proposed as a model to study heat transfer in micro heat pipes. The dual-wet pipe has a long and narrow cavity. The bottom-half of the horizontal pipe is made of a wetting material and holds a wetting liquid, whereas the top-half is made of a non-wetting material and is filled with the vapor. As one end of the pipe is heated, the liquid evaporates and increases the vapor pressure. The higher pressure drives the vapor to the cold end where the vapor condenses and releases the latent heat. The condensate moves along the bottom half of the pipe back to the hot end to complete the cycle. Hence, the heat pipe is driven by the difference in equilibrium vapor pressure between the hot and cold ends, and not by the liquid-vapor interfacial curvature as is commonly believed. Our analysis provides an explanation for the comparatively low effective thermal conductivity in micro heat pipes [1].
[1] Zhang, Watson & Wong, J. Fluid Mech. **589**, 1 (2007)

8:36AM P9.00004 Measuring velocity profiles and nanoparticle interactions between 20 and 300 nm from surfaces , PATRICK TABELING, CEDRIC BOUZIGUES, ESPCI, MICROFLUIDICS TEAM — The observation of flows at a nanometric scale is crucial for understanding phenomena involving interactions between liquids and solid surfaces, such as slippage and electro-osmosis. Here we report a new method based on nanoparticle imaging by total internal reflection fluorescence, allowing the first observation of water flows between 20 and 300 nm from surfaces. We probed the energy landscape, leading to first local measurements of the Debye length and surface/nanoparticle interactions; and provide an unambiguous determination with 10 nm accuracy of the slip length for different surfaces - wetting, non-wetting, hard, soft. These results represent an improvement of one order of magnitude compared to the state of the art. In addition to investigating locally energetic and electrostatic properties of the wall/liquid system, this Letter lays down the foundations of a technique that can foster the development of nanofluidics: Imaging of Nanoparticles for Energy landscape and Speed flow measurements (INES).

8:48AM P9.00005 Poisson-Nernst-Planck model of ion current rectification through a nanofluidic diode , DRAGOS CONSTANTIN, ZUZANNA SIWY, University of California, Irvine — We have investigated ion current rectification properties of a recently prepared bipolar nanofluidic diode. This device is based on a single conically shaped nanopore in a polymer film whose pore walls contain a sharp boundary between positively and negatively charged regions. A semiquantitative model that employs Poisson and Nernst-Planck equations predicts current-voltage curves as well as ionic concentrations and electric potential distributions in this system. We show that under certain conditions the rectification degree, defined as a ratio of currents recorded at the same voltage but opposite polarities, can reach values of over 1000 at a voltage range (-2V, +2V). The role of thickness and position of the transition zone on the ion current rectification is discussed as well. We also show that the rectification degree scales with the applied voltage.

9:00AM P9.00006 Non-reflecting boundary conditions for fluctuating hydrodynamics of compressible fluids , RAFAEL DELGADO-BUSCALIONI, Universidad Autonoma de Madrid, ANNE DEJOAN, CIEMAT, Madrid — Many important phenomena in microfluidics involve propagation of fast sound waves. Computational modeling of such problems requires a way to evacuate the reflected waves out of the computational box. However, a way to construct open boundary conditions for Fluctuating Hydrodynamics (FH) is lacking in the literature. This work presents open boundary conditions for fluctuating hydrodynamics solvers based on the Navier-Stokes Landau-Lifshitz equations. The objectives are i) ensure robust non-reflecting boundary conditions and ii) keep thermodynamic consistency for total mass fluctuation, i.e. agreement with the grand canonical ensemble. We show that by ensuring the fluctuation-dissipation balance for the total mass, one also gets the correct equilibrium power spectra of local mass and momentum at each point of the computational box. We consider real compressible fluids (argon and water) under isothermal condition and present results for the equilibrium and several out-of-equilibrium states involving generation of sound waves.

9:12AM P9.00007 ABSTRACT WITHDRAWN –

9:24AM P9.00008 Liquid precursor films spreading on chemically patterned substrates[1] , ANTONIO CHECCO, Condensed Matter Physics and Materials Science Dept, Brookhaven National Laboratory — We study the spreading of nonvolatile liquid squalane on chemically patterned nanostripes by using non-contact Atomic Force Microscopy (NC-AFM). The substrates are octadecylthrichlorosilane(OTS)-coated silicon wafers chemically patterned on multiple length-scales using a combination of UV and AFM oxidative lithographies. This process allows us to locally convert the terminal methyl groups of the OTS surface (non-wettable) into carboxylic acid groups (wettable) without affecting considerably the substrate roughness ($<$ 0.3nm rms). The patterned regions are shaped as a network of large (mm-sized) wettable lines connected to smaller and smaller (nm-sized) lines. Liquid squalane spreads across this "microfluidic network" starting from the large lines eventually reaching the nanolines (50 to 500 nm-wide). NC-AFM is used to image the morphology of the liquid as it spreads across the nanolines. We find that the liquid thickness on the nanolines grows with time (up to $\sim$10 nm) according to a power-law with exponent $\sim$1. These preliminary results suggest that the spreading dynamics of laterally-confined liquids slightly differs, as expected, from the one of laterally homogeneous precursor films. We compare our findings to recent theoretical predictions of confined liquid flow and also discuss its relevance to nanofluidics.

[1]supported by U.S. DOE under contract No. DE-AC02-98CH10886

9:36AM P9.00009 Velocity Dependent Selectivity of Deterministic Lateral Displacement Arrays[1] , JASON PUCHALLA, KEITH MORTON, ROBERT AUSTIN, Princeton University — Deterministic lateral displacement (DLD) has been demonstrated as a promising microfluidic method to circumvent diffusive dispersion while separating small particles based on size. At low average flow velocity, steric repulsion and diffusion seem sufficient to describe particle behavior and array separation characteristics. However, at higher but still laminar flow velocities, particle behavior changes drastically. We have investigated this regime using a silicon DLD array. We present how the local disruption of fluid flow about a moving particle and the effects inertial forces can alter DLD behavior and can be exploited for selective sorting.

[1]This work supported by DARPA W911NF-05-1-0392

9:48AM P9.00010 Fluctuation effects and evolution in bacterial populations on a chip , JAAN MANNIK, JUAN E. KEYMER, CEES DEKKER, Delft University of Technology — Fluctuation effects are ubiquitous in physics. Relatively little is known what role these effects play in systems involving biological organisms. How do random fluctuations originating from the environment and from the biological organisms itself affect the population dynamics and evolution? Here, we address this question using an experimental approach where we grow a large number of independent E. coli populations on a microfluidic silicon chip designed to evolve the body size distribution. We provide the same environmental conditions for different populations and follow their evolution in real time measuring number of bacteria in different colonies. We analyze fluctuations in these numbers and how the body size distribution of bacteria changes.

10:00AM P9.00011 Modelling colloidal dynamics in complex systems , CHRISTOPHER SMITH, COLIN DENNISTON, University of Western Ontario — We present a lattice Boltzmann method for dealing with solid moving boundaries in a fluid. A novel method is introduced to distribute a solid surface onto the fluid mesh. We show that for a single particle in a chute with Stokes flow, the quantitatively correct Stokes drag is obtained. Comparing two scenarios at the same Reynolds number, where the walls induce the flow or where the particle is moving, we show there is little discernible difference in the force measured. Next, we have a system with two particles and show we get quantitative agreement for the interaction between the two particles measured by our algorithm and the interaction expected according to the Rotne-Prager (RP) tensor or the Oseen tensor, in the regimes in which they are expected to be accurate. Moving away from irrotational flow, for a cylinder in a two dimensional chute the Reynolds number of the flow is increased further into the laminar region and we show the formation of eddies shedding off the solid surface. We incorporate this new algorithm into liquid crystals simulations to look at novel colloidal interactions through topological defects.

10:12AM P9.00012 Experimental and Theoretical Studies of Electroosmotic Membrane Micropumps , ZULI XU, JIANYING MIAO, NING WANG, PING SHENG, Department of Physics and Institute of Nano Science and Technology, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China — Electroosmotic (EO) effect means fluid flow (through a porous medium) induced by an applied electric field E. EO pumps have the advantages of no moving parts and easily-controlled accurate flow rate at low applied voltages. We have fabricated nano-channel EO membrane pumps using anodic aluminum oxide (AAO) as the template [1]. The diameter of the uniform-sized nanochannels can range from 60-300nm, with a membrane thickness of 30-100 microns. The EO effect is enhanced by coating the nano-channels with silica. By using de-ionized water, the nanopump performance is shown to agree reasonably well with the theoretical model, with factors such as the ratio of the double layer thickness to channel diameter, channel geometry, and treatment of the AAO membranes playing important roles. With silica coating to the nanochannels, the nanopump can produce a maximum pressure of 1 atm and a maximum flow rate of 86,000μL/min·cm2 under an applied field of 0.94 V/μm. Besides DI water, the micropumps have also been tested to work well with salt, acid or base solution. [1] J.Y. Miao, Z.L. Xu, X.Y. Zhang, N. Wang, Z.Y. Yang, P. Sheng, submitted to Advanced Materials (Appeared online: 10.1002/adma.200700767).

10:24AM P9.00013 Investigation and Characterisation of Resizeable Nanopores in an Elastomeric Membrane , GEOFF WILLMOTT, Industrial Research Limited — Experimental and theoretical work relating to the development of resizeable synthetic nanopores will be presented. The nanopores, which are roughly conical, are formed by puncturing a relatively thick ($\sim$250 μm) elastomeric membrane with an STM tip. The aperture can be closed and the size can be dynamically controlled by stretching the elastomer [1]. Use of this technology presents a collection of interesting physical problems, covering topics that include the failure and mechanical properties of the elastomer, flow of ionic current through the aperture and particle sensing using the resistive pulse technique. Synthetic nanopores have potential applications in many fields, but especially relating to nanoscale sensing and diagnostic devices, and replication of ion channels in living cells. [1] S. J. Sowerby, M. F. Broom, G. B. Petersen, Dynamically Resizable Nanometre-Scale Apertures for Molecular Sensing, Sensors and Actuators B: Chemical 123 (1), pp. 325-330 (2007)

10:36AM P9.00014 The physics of densely-packed emulsions , DONALD M. AUBRECHT, Harvard University, DAVID F. MARRAN, DARREN R. LINK, RainDance Technologies, Inc., DAVID A. WEITZ, Harvard University — One strategy for microfluidic lab-on-a-chip applications is to use water droplets as tiny reaction vessels in a carrier stream of oil. As biochemical and cell-based experiments often require control over events that take place over a wide range of time scales, strategies need to be developed to ensure adequate timing without limiting droplet throughput. In general, longer time scales can be achieved by using longer channels or more densely packed droplets. Long channels become increasingly impractical at high throughputs for times exceeding tens of minutes, thus motivating work with densely packed droplets. Dense packing of droplets can be achieved by generating droplets on-chip, collecting them off-chip to allow the oil to drain, and re-injecting them back on-chip as a packed emulsion. This strategy is limited in that it only provides access to time scales in excess of hours. Moderate time scales can be accessed by removing carrier oil from the flow without removing the droplets. Here we present some of the physical principles governing how this can be implemented and discuss the flow of the resulting dense collections of droplets through microchannels.

Wednesday, March 12, 2008 8:00AM - 10:48AM –

Session P16 DBP DPOLY DFD: Focus Session: Cytoskeletal Dynamics and Cell Motility I

Morial Convention Center 208

8:00AM P16.00001 Actin Disassembly Mediated by Severing, Debranching, and Hydrolysis[1] , ANDERS CARLSSON, Washington University in St. Louis — For cells to respond effectively to their environment, the actin cytoskeleton must both assemble and disassemble rapidly in the presence of external cues. A great deal of theory has been focused on assembly, but disassembly has so far received less attention. The talk will describe two theoretical treatments of actin disassembly resulting from debranching, severing, and ATP hydrolysis. 1) The dynamics of *in vitro* actin polymerization caused by filament branching or severing. Via a combination of stochastic-growth simulation and analytic theory, we show that highly branched structures such as those found near the edges of cells cannot persist in steady state. Early in polymerization, highly branched structures form, but disassemble over time leaving very few branched filaments. This causes an overshoot in light scattering intensity as a function of time. Inclusion of the effects of ATP hydrolysis shows that hydrolysis causes an overshoot in the amount of polymerized actin which can be observed in pyrene fluorescence experiments. 2) The interaction between severing and annealing in disassembling a model lamellipodial actin network. The network is treated as a periodic array of crosslinked actin filaments which sever randomly. The lamellipodial actin density drops abruptly as a function of distance from the membrane in the absence of annealing. When annealing is included, the drop is more gradual, and at a critical value of the annealing rate the thickness becomes infinite. It is shown that lamellipodial disassembly is controlled by two characteristic times: the time that a single subunit remains in the network, and the time that it takes for actin polymerized at the membrane to move to the edge of the lamellipodium.

[1]Supported by the National Science Foundation under grant DMS-0240770

8:36AM P16.00002 A Possible Role for a Viscous Fingering-Type Instability in Cell Motility , ANDREW CALLAN-JONES, JEAN-FRANCOIS JOANNY, Institut Curie-Phyiscal Chemistry Laboratory, JACQUES PROST, Institut Curie-Phyiscal Chemistry Laboratory/ESPCI — We present a novel flow instability that can arise in thin films of cytoskeletal fluids if the friction with the substrate on which the film lies is sufficiently strong. The motivation for this work are the experiments of Verkhovsky et al. (Verkhovsky et al, Curr. Biol., 9: 11-20 (1999)) in which flat, circular, stationary cell fragments on a substrate, containing only actin and myosin motors, can either spontaneously or under applied force change shape and start moving. In the stationary state in our model, actin polymerizes at the fragment edge and depolymerizes uniformly in the bulk. The initial velocity profile is radial and is imposed by mass conservation for constant polymer density. The radius of the fragment is fixed by conservation of total — monomer and filamentous—actin. Performing a linear stability analysis of the actin velocity due to perturbations of the fragment boundary, we find that as the dimensionless parameter $\frac{\eta}{\xi R_0^2} \to 0$, where ξ is the actin-substrate friction, η is the viscosity, and R_0 is the initial fragment radius, the perturbed velocity obeys a Darcy Law, and combined with the force-free condition at the fragment boundary, this leads identically to a viscous fingering instability. This asymptotic limit should be achievable since R_0 can be tuned by making a fragment with enough actin.

8:48AM P16.00003 The Stochastic Dynamics of Filopodial Growth[1] , GAREGIN A. PAPOIAN, YUEHENG LAN, PAVEL ZHURAVLEV, The University of North Carolina at Chapel Hill — A filopodium is a cytoplasmic projection, exquisitely built and regulated, which extends from the leading edge of the migrating cell, exploring the cell's neighborhood. Commonly, filopodia grow and retract after their initiation, exhibiting rich dynamical behaviors. We model the growth of a filopodium based on a stochastic description which incorporates mechanical, physical and biochemical components. Our model provides a full stochastic treatment of the actin monomer diffusion and polymerization of each individual actin filament under stress of the fluctuating membrane. We have investigated the length distribution of individual filaments in a growing filopodium and studied how it depends on various physical parameters. The distribution of filament lengths turned out to be narrow, which we explained by the negative feedback created by the membrane load and monomeric G-actin gradient. We also discovered that filopodial growth is strongly diminished upon increasing retrograde flow, suggesting that regulating the retrograde flow rate would be a highly efficient way to control filopodial extension dynamics. The filopodial length increases as the membrane fluctuations decrease, which we attributed to the unequal loading of the mem- brane force among individual filaments, which, in turn, results in larger average polymerization rates. We also observed significant diffusional noise of G-actin monomers, which leads to smaller G-actin flux along the filopodial tube compared with the prediction using the diffusion equation.

[1]This work was supported through National Science Foundation (NSF) grant 0715225.

9:00AM P16.00004 Mechanics of Lamellipodia , D. A. QUINT, J. M. SCHWARZ, Syracuse University — The actin cytoskeleton is a morphologically-complex assembly of cross-linked F-actin filaments. The cytoskeleton provides rigidity for the cell within appropriate time scales so that it can change its shape to, for example, crawl along surfaces. In addition to cross-linking proteins, many other proteins are involved in the assembly of the actin cytoskeleton such as branching proteins, capping proteins, and severing proteins. Presumably these proteins work cooperatively toward the dynamic formation of rigidity. We will initially focus on the role of branching proteins. The F-actin filaments in lamellipodia—protrusions of the mobile edge of a crawling cell—have some overall orientation due to the branching. Branched filaments emerge at a 70 degree angle from the mother filament's growing end.[1] This overall orientation is modelled as an anisotropy in an effective medium theory determining the cytoskeleton's elasticity in the static regime. The potential for a splay rigid phase, in addition to a rigid phase, is also investigated.

[1]T. M. Svitkina and G. G. Borisy, *J. Cell Biol.* **145**, 1009 (1999).

9:12AM P16.00005 Assembly Mechanism of the Contractile Ring for Cytokinesis by Fission Yeast , DIMITRIOS VAVYLONIS, Lehigh University, JIAN-QIU WU, Ohio State University, XIAOLEI HUANG, Lehigh University, BEN O'SHAUGHNESSY, Columbia University, THOMAS POLLARD, Yale University — Animals and fungi assemble a contractile ring of actin filaments and the motor protein myosin to separate into individual daughter cells during cytokinesis. We studied the mechanism of contractile ring assembly in fission yeast with high time resolution confocal microscopy, computational image analysis methods, and numerical simulations. Approximately 63 nodes containing myosin, broadly distributed around the cell equator, assembled into a ring through stochastic motions, making many starts, stops, and changes of direction as they condense into a ring. Estimates of node friction coefficients from the mean square displacement of stationary nodes imply forces for node movement are greater than $\sim$ 4 pN, similarly to forces by a few molecular motors. Skeletonization and topology analysis of images of cells expressing fluorescent actin filament markers showed transient linear elements extending in all directions from myosin nodes and establishing connections among them. We propose a model with traction between nodes depending on transient connections established by stochastic search and capture ("search, capture, pull and release"). Numerical simulations of the model using parameter values obtained from experiment succesfully condense nodes into a continuous ring.

9:24AM P16.00006 Nonlinear elasticity of composite networks of stiff biopolymers with flexible linkers , CHASE BROEDERSZ, Vrije Universiteit, C. STORM, Vrije Universiteit and Universiteit Leiden, F.C. MACKINTOSH, Vrije Universiteit — Motivated by recent experiments showing novel rheological properties of biopolymer networks, we develop an effective medium theory for rigid filaments cross-linked by flexible linkers. Specifically, we treat such a network as a collection of randomly oriented stiff polymers mechanically connected by highly compliant cross-linkers to an elastic continuum, which effectively represents the surrounding network. For cross-links with a finite compliance, we find a smooth cross-over between two distinct elastic regimes. Starting from a linear elastic regime dominated by cross-link elasticity, the network begins to stiffen significantly as the cross-links reach full compliance. We extend this model to a self-consistent one, in which the effective medium reflects the non-linear elastic properties of the cross-linked network. This model yields a cross-over to a nonlinear regime that is consistent with recent experimental studies of the cellular cytoskeletal polymer F-actinwith filamin cross-links[1].

1. ML Gardel, F Nakamura, J Hartwig JC Crocker, TP Stossel, DA Weitz, **103**, 1762 Proc. Nat. Ac. Sci. (2006).

9:36AM P16.00007 Effects of Osmotic Force and Torque on Microtubule Bundling and Pattern Formation , YONGXING GUO, YIFENG LIU, Physics Department, Brown Univ., RUDOLF OLDENBOURG, Marine Biological Laboratory, JAY TANG, JAMES VALLES, Physics Department, Brown Univ. — We report the effect of Polyethylene Glycol (PEG, MW=35kd) on microtubule bundling and pattern formation. Without PEG, polymerizing microtubule (MT) solutions of a few mg/ml [1,2] can spontaneously form striated birefringence patterns through MT alignment, bundling and buckling in coordination. With PEG, bundles become more distinct and the birefringence pattern weakens. Using quantitative birefringence measurements, the average number of MTs in the cross section of a bundle induced by 1% w/w PEG 35kd is determined to be around 26, with a wide spread in size. The amplitude of the buckling is reduced with increased PEG concentration. At sufficiently high PEG concentration ($\sim$0.5% w/w), the pattern is totally suppressed and the sample contracts laterally during the development of a microtubule bundle network. We propose that the decrease of the buckling amplitude is due to the depletion of the dispersed MT network, which is essential for the pattern formation. We attribute the anisotropic contraction to an osmotic torque that drives bundles that cross to align. [1] Y. Liu, *et al.*, PNAS 103, 10654 (2006). [2] Y. Guo, *et al.*, PRL 98, 198103 (2007). [Supported by NASA (NNA04CC57G, NAG3-2882) and NSF (DMR 0405156)]

9:48AM P16.00008 Buckling and force propagation in intracellular microtubules , MOUMITA DAS, Vrije Universiteit, ALEX J. LEVINE, University of California, Los Angeles, F.C. MACKINTOSH, Vrije Universiteit — Motivated by recent experiments [1] showing the buckling of microtubules in cells, we study theoretically the mechanical response of, and force propagation along elastic filaments embedded in a non-linear elastic medium. We find that embedded microtubules buckle when their compressive load exceeds a critical value f_c which is two orders of magnitude larger than for an isolated MT as found earlier [1], and that the resulting deformation is restricted to a penetration depth that depends on both the non-linear material properties of the surrounding cytoskeleton, as well as the direct coupling of the microtubule to the cytoskeleton possibly through MT-associating proteins (MAPS). The deformation amplitude depends on the applied load $f > f_c$ as $(f - f_c)^{1/2}$. This work shows how the range of compressive force transmission by microtubules can be as large as tens of microns, and is governed by the mechanical coupling to the surrounding cytoskeleton.

References:
[1] CP Brangwynne et al., J. Cell Biology, 173, 733 (2006).

10:00AM P16.00009 Hydrodynamic tether extrusion from "gelly" vesicles , KARINE GUEVORKIAN, SEBASTIEN KREMER, FRANCOISE BROCHARD-WYART, Institut Curie — Extrusion of cell tethers requires the detachment of the plasma membrane and can be used to probe the strength of membrane-cytoskeleton adhesion. We have studied the hydrodynamic extrusion of tethers from red blood cells [1] and developed a theoretical model based on permeation of lipids through the network of membrane proteins linked to the cytoskeleton [2]. Our aim here is to probe the model on biomimetic systems, namely lipid vesicles filled with artificial cytoskeleton made of synthetic or biological gels, where we can adjust the membrane-cytoskeleton coupling. The properties of tubes extruded from these "gelly" vesicles will be compared to simple vesicles on one hand, and to red blood cells or human carcinoid BON cells on the other. [1] N. Borghi et al, Biophys. J. 93 (2007) [2] F. Brochard-Wyart, et al, Proc. Natl. Acad. Sci. USA, 103 (2006)

10:12AM P16.00010 Living Microlens Arrays[1] , JESSICA ZIMBERLIN, PATRICIA WADSWORTH, ALFRED CROSBY, University of Massachusetts — Using the properties of living cells and early tissue formation, we define adaptable surface structures of three-dimensional, hexagonal arrays of microlenses. These "living" microlenses are achieved by growing a monolayer cell sheet on a thin film of polystyrene [PS] attached to a substrate of crosslinked poly(dimethyl siloxane) [PDMS] microwells. The contractile nature of the cells attached to the surface and the compliance of the PDMS surface geometry allows the PS thin film to buckle, forming arrays of convex microlenses. The curvature of the microlens structures is related to the strain applied by monolayer cell sheets to the PS surface. We use this measurement to differentiate the strains applied by two different cell types and relate these strains to differences in the intercellular coupling of the different cell types. We also show that by adding different chemical triggers to the system, the contractile nature of the cells changes, modifying the focal length of the microlenses. This design introduces a new paradigm for advanced materials and offers great promise for a range of applications.

[1]Authors would like to acknowledge NSF-IGERT and NIH for their support.

10:24AM P16.00011 Local viscoelasticity of the surfaces of individual Gram-negative bacterial cells measured using atomic force microscopy , VIRGINIA VADILLO-RODRIGUEZ, TERRY BEVERIDGE, JOHN DUTCHER, University of Guelph — The cell wall of Gram-negative bacteria performs many important biological functions: it plays a structural role, it allows the selective movement of molecules across itself, and it allows for growth and division. These functions not only suggest that the cell wall is dynamic, but that its mechanical properties are very important. We have used a novel, AFM-based approach to probe the mechanical properties of single bacterial cells by applying a constant compressive force to the cell under physiological conditions while measuring the time-dependent displacement (creep) of the AFM tip due to the viscoelastic properties of the cell. For these experiments, we chose a representative Gram-negative bacterium, *P. aeruginosa* PAO1, and we used AFM tips of different size and geometry. We find that the cell response is well described by a three element mechanical model with an effective cell spring constant k and an effective time constant τ for the creep motion. Adding glutaraldehyde, which increases the covalent bonding of the cell surface, produced a significant increase in k and a significant decrease in τ.

10:36AM P16.00012 Stall Force and Response of Lung Cilia , RICHARD SUPERFINE, DAVID HILL, VINAY SWAMINATHAN, E. TIMOTHY O'BRIEN, University of North Carolina, RIC BOUCHER, BRIAN BUTTON, ASHLEY ESTES — We report on the response of lung cilia to applied forces. We have applied magnetic forces to magnetic beads attached to individual human lung cilia in cell cultures. Our magnetic system is capable of generating large forces ($\sim$1nanoNewton on 1 micron beads) with a 3kHz bandwidth. We record the cilia beat motion using video microscopy to record beat frequency and amplitude as a function of applied force. We present three major findings. First, the stall force is approximately 150 pN. Second the frequency is unchanged by the application of forces up to the stall point. Third, the speed of the beat motion slows down according to the diminution of the beat amplitude while maintaining a constant frequency and the speed of the motion is the same whether the beat direction is in the same direction as the applied force or against the applied force.

Wednesday, March 12, 2008 11:15AM - 2:15PM –

Session Q8 DFD: Colloidal Phase Behavior Morial Convention Center RO6

11:15AM Q8.00001 Studies of colloids on spherical interfaces using digital holographic microscopy , JEROME FUNG, RYAN J. MCGORTY, VINOTHAN N. MANOHARAN, Harvard University, Dept. of Physics — Colloidal particles pinned to the surface of an oil droplet in water form robust equilibrium structures at low area fractions. To better understand the interactions in this system, we are studying these structures and their dynamics during quasistatic changes in the area fraction. We do so by imaging the 3D structures with fast temporal resolution using digital holographic microscopy (DHM). To keep the particles in non-density matched colloidal samples in the field of view, we have constructed a new apparatus to perform DHM under time-averaged zero gravity using a rotating stage. In DHM, we illuminate a sample with a laser beam and then magnify and digitally record the interference patterns between the scattered and unscattered light. Subsequent numerical reconstruction of the recorded 2D holograms allows 3D particle tracking with millisecond time resolution and submicron spatial resolution.

11:27AM Q8.00002 Confinement Finds a Length Scale for the Colloidal Glass Transition , KAZEM EDMOND, ERIC R. WEEKS, Emory University — We study a colloidal suspension confined between two parallel walls as a model system for glass transitions in confined geometries. We use confocal microscopy to directly observe the motion of the colloidal particles, which are slower when confined. This slower motion produces glassy behavior in a sample that is liquid-like when not confined. Our results, from a range of volume fractions, demonstrate that the maximum thickness where confinement is effective defines a length scale for a given particle volume fraction. The length scale increases as the glass transition is approached. We observe that near the glass transition particle motion is strongly spatially correlated. We investigate the relationship between the length scales of these correlations and the established confinement length scale.

11:39AM Q8.00003 Dislocation nucleation and motion observed in a 2D Yukawa triangular lattice , V. NOSENKO, S. ZHDANOV, G. MORFILL, Max-Planck-Institute for extraterrestrial Physics — Dislocation nucleation and motion were studied experimentally in a 2D Yukawa triangular lattice. Edge dislocations were created in pairs in lattice locations where the internal shear stress exceeded a threshold and then moved apart in the glide plane at a speed higher than the sound speed of shear waves. The early stage of this process is identified as a stacking fault. At a later stage, supersonically moving dislocations generated shear-wave Mach cones. The experimental system, a plasma crystal, allowed observation of this process at an atomistic (kinetic) level. We used a monolayer suspension of microspheres in a plasma, i.e., a complex plasma, which is like a colloidal suspension, but with an extremely low volume fraction and a partially-ionized rarefied gas instead of solvent. At our experimental conditions, the suspension forms a highly ordered 2D triangular lattice. Dislocations were generated in this lattice due to the shear introduced by its differential rotation, with two "rigid" domain walls imbedded in it. We used digital video microscopy for direct imaging and particle tracking.

11:51AM Q8.00004 Low-electric-field phase behaviour of Brownian colloidal suspensions in sedimentation equilibrium[1] , AMIT AGARWAL, NING LI, ANAND YETHIRAJ, Department of Physics and Physical Oceanography, Memorial University of Newfoundland — We study the phase diagram of the suspension of micron-scale fluorescent labeled silica colloids in aqueous suspension as a function of concentration in the presence of a moderate (less than 1 volt per μm) AC electric field. Confocal microscopy was used to track three-dimensional structure and dynamics of colloidal suspensions in sedimentation equilibrium. We characterize thresholds for field-induced organization in monodisperse colloidal suspensions of two particle diameters using orientational order parameters. We then study structure formation at moderate fields above the field threshold. At concentrations greater than 10%, and electric fields much larger than the field threshold measured, the colloidal suspension crystallizes to form a body centered tetragonal structure as has been previously reported. At lower concentrations and moderate fields, we uncover complex structure formation phenomena that include equilibrium cellular structures.

[1]This work is supported by NSERC (Canada).

12:03PM Q8.00005 Benchmarks for simulations of colloidal suspensions[1] , TONY LADD, University of Florida — There are now a number of methods available to investigate the dynamics of colloidal suspensions; among the most popular are Stokesian dynamics, the lattice-Boltzmann equation, dissipative particle dynamics, and stochastic rotation dynamics. One of the most commonly asked questions is how do the various methods compare in terms of accuracy and computational cost. At present there is no meaningful answer, in part because it is not straightforward to construct clean test calculations and obtain reference solutions to these problems. I will outline some principles that may be helpful in developing a basis for comparison and describe preliminary results obtained with the lattice-Boltzmann method.

[1]This work was supported by the National Science Foundation (CTS-0505929)

12:15PM Q8.00006 Non-equilibrium Crystallization Kinetics of an Induced Transition Observed in a Nano-Colloidal Liquid Crystal-Aerosil Dispersions[1] , DIPTI SHARMA, Worcester Polytechnic Institute — A new transition feature, termed "Induced Crystallization" (IC), has been observed in a nano-colloidal liquid crystal (octylcyanobiphenyl, 8CB) and aerosil gel system dependent on silica content. This IC feature exhibits apparent activated kinetics following Arrhenius-like behavior. Temperature scans were performed on heating using a DSC technique at ramp rates from 1 to 20 K/min and the aerosil density varied from 0 to 0.2 g/cc. For the 8CB+sil, a well resolved exothermic peak was found as an additional feature on heating scan before the melting transition, absent in bulk 8CB. As the sil density increases, the observed the enthalpy increases while the effective activation energy decreases for this IC feature, eventually saturating at the highest density studied. This behavior appears consistent with molecular disorder imposed by the surface molecular interaction, inducing slow glassy crystallization of the 8CB liquid crystal.

[1]Author is grateful to Germano Iannacchione for many useful discussions.

12:27PM Q8.00007 Phase separation in asymmetric 2D binary hard-sphere mixtures[1] , CAMILO GUAQUETA, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — We investigate the phase behavior and structural properties of highly asymmetric binary mixtures of additive hard spheres in two dimensions, using Monte Carlo simulations in both the canonical and restricted Gibbs ensembles. To tackle large diameter ratios between the large and small species we use an efficient geometric cluster algorithm. Results for the pair correlation functions, compressibility, and depletion potentials are presented and compared to theoretical predictions, for diameter ratios from $q = 2$ to $q = 400$ and over a wide range of packing fractions. We explore and comment on the possibility of a demixing transition at high q and total packing fraction.

[1]This work is supported by the National Science Foundation through Grant No. DMR-0346914.

12:39PM Q8.00008 Experiments on a two dimensional lattice of charged colloids above a water-oil interface , WILLIAM IRVINE, YAEL ROICHMANN, ANDREW HOLLINGSWORTH, DAVID GRIER, PAUL CHAIKIN, Department of Physics and Center for Soft Matter Research, New York University — Charged hydrophobic (PMMA) colloids in an oil phase (cyclohexyl bromide) are attracted, without wetting, by image charge effects to an oil-water interface. The micron size spheres form a monolayer on the interface and interact via screened coulomb interactions to form a crystalline or hexatic lattice, depending on the tunable ratio of lattice spacing to screening length. We study the statics and dynamics of this system in periodic, commensurate, incommensurate, random and quasi-periodic potentials applied by holographic optical tweezers. The use of holographic tweezers allows considerable control over the character and strength of the applied potential. A similar system has been used to study the effects of a curved fluid interface on the particle density and on topological defects.

12:51PM Q8.00009 Nematic Order on Foams , BRYAN CHEN, RANDALL KAMIEN, University of Pennsylvania — We investigate the competition between nematic order and area minimization in nematic foams, in particular, how the structure is affected by the bending of the nematic director, and whether these systems will continue to obey Plateau's laws. We study the minimum energy configurations of the director field on a one parameter family of perturbed Reuleaux tetrahedra with special attention to the location of topological defects. We determine the energy distribution at the Plateau borders versus the film surface and relate the change in structure to changes in elastic constants and surface tension.

1:03PM Q8.00010 Restricted Defect Dynamics in Colloidal Peanut Crystals , SHARON GERBODE, Physics - Cornell University, STEPHANIE LEE, Materials Science and Engineering - Cornell University, BETTINA JOHN, Chemical Engineering - Cornell University, ANGIE WOLFGANG, Physics - Cornell University, CHEKESHA LIDDELL, Materials Science and Engineering - Cornell University, FERNANDO ESCOBEDO, Chemical Engineering - Cornell University, ITAI COHEN, Physics - Cornell University — We report that monolayers of hard peanut-shaped colloidal particles consisting of two connected spherical lobes order into a crystalline phase at high area fractions. In this "lobe-close-packed" (LCP) crystal, the peanut particle lobes occupy triangular lattice sites, much like close-packed spheres, while the connections between lobe pairs are randomly oriented, uniformly populating the three crystalline directions of the underlying lattice. Using optical microscopy, we directly observe defect nucleation and dynamics in sheared LCP crystals. We find that many particle configurations form obstacles blocking dislocation glide. Consequently, in stark contrast to colloidal monolayers of close-packed spheres, single dislocation pair nucleation is not the only significant energetic barrier to relieving an imposed shear strain. Dislocation propagation beyond such obstructions can proceed only through additional mechanisms such as dislocation reactions. We discuss the implications of such restricted defect mobility for the plasticity of LCP crystals.

1:15PM Q8.00011 Two-dimensional Dimer System , XIAOCHAO XU, DAVID PINE, Dept. of Physics and CSMR, New York University — We report on an experimental study of the two-dimensional phase behavior of colloidal dumbbells (dimers) trapped at a water-air interface. The dimers are made out of $1.6\,\mu$m silica microspheres that are fused together at a point. The water-air interface is very slightly concave so that the dimers are gently compressed by gravity towards the center of interface. The spheres form a stable dense state after a few days. For this dense phase, the location of peaks of both positional and angular pair correlation functions of the dimers reveals that many different orientations and configurations of the dimers are present and this is in agreement with the disorder crystal phase predicted by Monte Carlo Simulation. [1] We found that there is a relatively long range angular correlation, but the positional correlation is short-ranged. This long range angular correlation is limited by the domain sizes which are determined by the density of the defects in the system.

[1] K. W. Wojciechowski, A. C. Brańka and D. Frenkel, Physica A **196**, 519 (1993).

1:27PM Q8.00012 Observing liquid-gas nucleation in a colloid-polymer solution using digital holographic microscopy , RYAN MCGORTY, VINOTHAN N. MANOHARAN, Harvard University — We study liquid-gas nucleation in a colloid-polymer solution. Though the colloidal particles are too small to resolve, we are able to observe nucleating droplets due to the refractive index mismatch between the two fluid phases. By using digital holographic microscopy we are able to observe the three-dimensional structure of the nucleating phase. The experimental setup and algorithms for reconstructing the holography data will be discussed. We hope that our data will allow us to better understand nucleation kinetics and that analysis of the fluctuating droplets will provide us with the surface tension between the two phases.

1:39PM Q8.00013 Soft Spheres Make More Mesophases , CHRISTIAN SANTANGELO, Department of Physics, University of Massachusetts, Amherst, MA 01003, MATTHEW GLASER, Department of Physics, University of Colorado, Boulder, CO 80309-0390, USA, GREGORY GRASON, Department of Polymer Science, University of Massachusetts, Amherst, MA 01003, USA, RANDALL KAMIEN, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19004, USA, ANDREIJ KOSMRLJ, Massachusetts Institute of Technology, Cambridge, MA 02139-4307, USA, PRIMOZ ZIHERL, Department of Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia — We use both mean-field methods and numerical simulation to study the phase diagram of classical particles interacting with a hard-core and repulsive, soft shoulder. Despite the purely repulsive interaction, this system displays a remarkable array of aggregate phases arising from the competition between the hard-core and shoulder length scales. In the limit of large shoulder width to core size, we argue that this phase diagram has a number of universal features, and classify the set of repulsive shoulders that lead to aggregation at high density. Surprisingly, the phase sequence and aggregate size adjusts so as to keep almost constant inter-aggregate separation.

1:51PM Q8.00014 Correlations between Dynamical Heterogeneities and Visco-elastic properties of Confined Colloidal Thin Films , PRASAD SARANGAPANI, Y. ELAINE ZHU, University of Notre Dame, Department of Chemical and Biomolecular Engineering, Notre Dame, IN 46556 — Our recent study on confined hard-sphere colloidal suspensions demonstrates that glass transition can be observed 'sooner' as film thickness approaches a critical value while volume fraction remains constant. In this talk, we present a new study of the rheological properties of strongly confined colloidal thin films by using a home-designed micro-rheometer interfaced with a confocal microscope. We visualize the shear-induced structural relaxation at a single particle level and measure the rheological properties of confined colloidal thin films between two surfaces at narrow gap spacing ranging from 50 μm to 1-2 μm. The application of shear excitation greatly accelerates structural relaxation compared to quiescent colloidal fluids and we visualize particle displacements during the "bond breakage" process in strongly confined thin films. Additionally, we characterize their patterns, size and lifetimes under varied shear rates, and correlate their behaviors to the measured visco-elastic and visco-plastic properties of confined colloidal thin films.

2:03PM Q8.00015 Direct Imaging of the Collapsed Langmuir Monolayers and Multilayer Formation , DOSEOK KIM, Department of physics and Interdisciplinary Program of Integrated Biotechnology, Sogang University, SANGJUN SEOK, Department of Physics, Sogang University, TAE JUNG KIM, YOUNG DONG KIM, Nano-Optical Property Laboratory and Department of Physics, Kyung Hee University, DAVID VAKNIN, Ames Laboratory, Iowa State University — *In-situ* ellipsometry imaging was used to monitor Langmuir monolayer of arachidic-acid spread on water and on $CaCl_2$ solution before and after collapse. The Langmuir monolayer was collapsed by compressing it beyond the minimal closely-packed surface molecular area. The ellipsometry image showed clear domains of collapsed regions, and analysis of the image allowed determination of thicknesses of these domains. It was found that the structure of multilayer domain in the collapsed region was bilayer of arachidic acid on the surface of $CaCl_2$ solution, while the trilayer was formed on the pure water surface.

Wednesday, March 12, 2008 11:15AM - 2:03PM –

Session Q9 DFD: Focus Session: DNA and Biofluid Analysis with Micro and Nanofluidic Devices

Morial Convention Center RO7

11:15AM Q9.00001 Using hydrodynamics to control DNA conformation for genotyping, sorting, and analysis , SUSAN MULLER, Univ. of California, Berkeley — Understanding the dynamics of biopolymers in complex flows is critical for the successful design of lab-on-a-chip devices. Work by Chu, Shaqfeh, and others using both Brownian dynamics simulations and direct, single molecule visualization methods have yielded unprecedented insights into DNA dynamics in simple shear, planar extension, and a range of linear mixed flows. Here, we focus on two flows designed to stretch and manipulate DNA conformation for single molecule genotyping and analysis; that is, flows designed to produce specific conformation fields. First, we present results on DNA in pressure-driven flow through a post array, and discuss insights from direct comparisons with Brownian Dynamics simulations by Shaqfeh and co-workers. Second, we consider stagnation point flows and, through the use of sequence-specific probes, demonstrate the potential of these flows for target sequence identification, single molecule studies of enzyme kinetics, and sorting.

11:51AM Q9.00002 Droplet-based microfluidics for high-throughput scanning of a large probe library. , ADAM ABATE, DAVE WEITZ, Harvard University — Droplet-based microfluidics can produce monodisperse picoliter size microreactors at 10 kHz speed. We use this technology to prepare and fuse two drop trains. The drops in one train each contain a unique biochemical probe. The drops in the other train contain a probe target, enzymes, proteins, and other biochemical reagents that are necessary to sufficiently mimic the cellular environment. We synchronize the trains hydrodynamically and use electro-coalescence to perform high-throughput controlled fusion of one of each type of droplet microreactor. Using a multicolor laser excitation and fluorescence polarization detector we monitor each fusion event to observe the state of the probe and extract information about the target. This allows us to scan through a large probe library in a matter of seconds using less than 1μL or reagent.

12:03PM Q9.00003 Distant-ion dragging of polarizable nanodroplets and solvated DNA on nanotubes , BOYANG WANG, PETR KRAL, University of Illinois at Chicago, PROF. KRAL'S RESEARCH GROUP TEAM — Long distance Coulombic coupling allows efficient molecular dragging at the nanoscale by moving electrons, ions and molecules [1]. We use molecular dynamics simulations to show that ions intercalated inside semiconducting single-wall carbon nanotubes (SWNT) can be solvated in polarizable nanodroplets adsorbed on the SWNTs, and the coupled systems can be dragged by electric fields [2]. We also demonstrate that solvated single-strand DNA molecules adsorbed on SWNTs can be driven by ionic solutions flowing inside the tubes. These phenomena could be applied in molecular delivery, separation, desalination and be integrated in modern lab-on-a-chip technologies. [1] Boyang Wang and Petr Kral, JACS 128, 15984 (2006). [2] Boyang Wang and Petr Kral, submitted.

12:15PM Q9.00004 Spontaneous and coherent Raman spectroscopy of microfluidic flows , RAJAN ARORA, GEORGI PETROV, VLADISLAV YAKOVLEV, University of Wisconsin-Milwaukee, UNIVERSITY OF WISCONSIN-MILWAUKEE TEAM — Identifying protein structure and understanding its conformational dynamics are the grand challenges for biomedical science. The advent and most recent progress of microfluidics holds a promise of successfully addressing the major issues of structure determination—protein crystallization—by greatly multiplexing the evaluated number of crystallization conditions and protein dynamics—protein folding—by achieving a microsecond scale mixing. The further success of these approaches will strangely depend on the availability of remote probes capable of non-invasive interrogating the structure of biological molecules. Vibrational spectroscopy offers superior structural and chemical sensitivity, which can be successfully applied for characterizing transitional kinetics in microfluidic channels. In particular Raman and CARS give the molecular fingerprint along with structural information that is not possible with conventional fluorescence measurements. Here we are investigating the potential applicability of spontaneous and coherent Raman spectroscopy for protein folding and crystallization. Under suitable experimental conditions coherent Raman is seen to be 100 times more efficient than conventional Raman.

12:27PM Q9.00005 Detection of Kinase Translocation Using Microfluidic Electroporative Flow Cytometry , CHANG LU, JUN WANG, NING BAO, LEELA PARIS, HSIANG-YU WANG, ROBERT GEAHLEN, Purdue University, West Lafayette, IN, BIOLOGICAL ENGINEERING COLLABORATION, PHARMACY COLLABORATION — Translocation of a protein between different subcellular compartments is a common event during signal transduction in living cells. Detection of these events has been largely carried out based on imaging of a low number of cells and subcellular fractionation/Western blotting. These conventional techniques either lack the high throughput desired for probing an entire cell population or provide only the average behaviors of cell populations without information from single cells. Here we demonstrate a new tool, referred to as microfluidic electroporative flow cytometry, to detect the translocation of an EGFP-tagged tyrosine kinase, Syk, to the plasma membrane in B cells at the level of the cell population. We combine electroporation with flow cytometry and observe the release of intracellular kinase out of the cells during electroporation. We found that the release of the kinase was strongly influenced by its subcellular localization. Cells stimulated through the antigen receptor have a fraction of the kinase at the plasma membrane and retain more kinase after electroporation than do cells without stimulation and translocation. This tool will have utility for kinase-related drug discovery and tumor diagnosis and staging.

12:39PM Q9.00006 DNA/Protein Concentration and Identification by Nano-Channel Electrokinetics , GILAD YOSSIFON, HSUEH-CHIA CHANG, University of Notre Dame — Electric field focusing into charged nano-channels can concentrate and filter charged biological molecules. This transport specificity is further enhanced with sequence or receptor specific DNA probes and antibodies functionalized onto the channel wall or nano-colloids. Our theoretical and experimental studies show, however, the same field-focusing phenomenon can discharge mobile ions from the channel and produce a growing polarized layer outside the channel, both of which can significantly affect the I-V characteristics and molecular migration rate within the channel. Conversely, the presence of trapped molecules or nano-colloids can be sensitively detected with nano-channel impedance spectroscopy due to such field-focusing phenomena. We present several DC and AC electrokinetic techniques for concentrating, filtering and detecting biomolecules in nano-channels based on this principle.

12:51PM Q9.00007 DNA dynamics in sub-persistence length confinement[1] , YENG-LONG CHEN, ARSEN GRIGORYAN, Institute of Physics, Academia Sinica — Recent advances in genomic science and microscopy have spurred extensive investigation of the dynamics of double stranded DNA molecules in bulk solution and micron- and nano-scale fluidic channels. On the length scale of the DNA molecule's radius of gyration, classical polymer physics has been extremely successful in predicting the macromolecule's conformation and dynamics. With the availability of sub-100nm channels, it has become possible to study with detail the conformation and dynamics of DNA at the length scale of the DNA persistence length ($\sim$50nm), as well as DNA interactions with other molecules such as proteins. We employ Brownian dynamics simulations to explore DNA dynamics confined in channels of the DNA persistence length scale. The bending and thermal energy, the conformational entropy, and the DNA-surface interactions all contribute to the macromolecular dynamics. We compare our simulation results to the predictions of the Odijk theory for confined polymers, and we find that the confinement strongly affects the chain conformation and dynamics and lead to non-monotonic extensional relaxation.

[1]Supported by National Science Council of Taiwan

1:03PM Q9.00008 Learning from the Jersey Turnpike:Cell Lysis, Labeling and Washing with Microfluidic Metamaterials[1] , KEVIN LOUTHERBACK, KEITH MORTON, DAVID INGLIS, Princeton University, OPHELI TSUI, Boston University, JAMES STURM, STEPHEN CHOU, ROBERT AUSTIN, Princeton University — Directing objects across functional streamlines at low Reynolds number is difficult but important since this motion can be used to label, lyse, and analyze complex biological objects on-chip without cross-contamination. Here we use an asymmeteric post array to move cells across coflowing reagents and show on-chip, immunofluorescent labeling of platelets with washing and *E.Coli* cell lysis with simultaneous separation of bacterial chromosome from the cell contents. Furthermore, we develop the concept of a microfluidic metamaterial by using the basic asymmetric post array as a building block for complex particle handling modes. These modular array elements could be of great use for developing robust techniques for on-chip, continuous flow manipulation and analysis of cells, large bio-particles, and functional beads.

[1]Supported by the AFOSR, NIH (HG01506), NSF Nanobiology Technology Center (BSCECS9876771.

1:15PM Q9.00009 Scaling of Polymer Diffusivity in Confined Colloid-Polymer Systems , AMIR AMINI, Rice University, MARC ROBERT, Rice Quantum Institute, and Richard E. Smalley Institute for Nanoscale Science and Technology, Rice University — We show how the diffusivity of a polymer chain in a colloidal suspension varies with the extent of confinement and the number of segments, as well as with concentration of colloids. These predications are compared with experimental results

1:27PM Q9.00010 Dynamics of Individual Flexible Biopolymers in a Microvortex Flow , CHAO-MIN CHENG, PHILIP LEDUC, Carnegie Mellon University, CARNEGIE MELLON UNIVERSITY TEAM — Research in single polymer dynamics has provided exciting insights including increasing the understanding of cellular structures. Additionally, advances in micro-scale technologies such as microfluidics have been widely used for analyzing biological responses at the cellular and molecular levels. We describe observations of the real-time dynamics of individual flexible polymers (fluorescently labeled DNA molecules) under a microvortex environment through a pressure-driven microfluidic approach. This allows us to create a microvortex flow on a single molecule, which can simultaneously be imaged to determine the structural response of the individual molecule. The DNA exhibits distinct conformations and controlled curvatures that are influenced by both extension and bending dynamics, which can be directly correlated to their location within the microvortex. We analyzed the dynamics of these individual molecules and determined the elongation strain rate and the curvature under the pressure-driven flow. Their overall orientation ranges from parallel in the main inlet channel to perpendicular while being deformed within the flow inside of the microvortex. These results provide insights that will be important in numerous areas such as single molecule dynamics and polymer physics.

1:39PM Q9.00011 Microfluidic devices for separation of human blood samples , VIRGINIA VANDELINDER, ALEX GROISMAN, UCSD — We describe design and operation of microfluidic devices for separation of human blood. The first device separates plasma from the cellular elements of blood using size exclusion in a cross-flow. The device generates 1 uL of high-quality plasma four minutes after loading the blood sample and can operate continuously for at least one hour. The second device separates white bloods cells (WBC) from red blood cells (RBC) using perfusion in a continuous cross-flow. The microfluidic device is tested with a suspension of polystyrene beads and is shown to efficaciously exchange the carrier medium while retaining all beads. The RBC content of the blood sample is reduced about 4000-fold while 98 percent of WBCs are retained with a resultant WBC : RBC ratio of 2.4 at the device outlet.

1:51PM Q9.00012 Cheaters and Cooperators: A Study of Bacterial Conflict on a Chip[1] , GUILLAUME LAMBERT, PETER GALAJDA, JUAN KEYMER, ROBERT AUSTIN, Princeton University — We study the interaction of cheating and cooperating *escherichia Coli* metapopulations under selective pressure on chip designed to create a landscape of metabolic pressures. Using micro- and nano-fabrication techniques, we create microfluidic chips with an effective 'fitness landscape' for the bacterial cells at the population level in which we can tune their access to spatial and energetic resources. Our custom-made micro habitats allow us to study the local density distribution and subpopulation dynamics of bacterial cells subjected to social pressure. We show that the microscopic collective behavior of the cheaters and cooperators differ greatly depending on the fitness landscape they evolved in. Locally, subpopulations emerge and compete in a 'tug-of-war' fashion. Globally, metapopulations rise, fall, evolve and adapt to their hostile environment.

[1]Supported by AFOSR, NIH (HG01506), NSF Nanobiology Technology Center (BSCECS9876771.

Wednesday, March 12, 2008 11:15AM - 2:15PM –

Session Q16 DBP DPOLY DFD: Focus Session: Cytoskeletal Dynamics and Cell Motility II

Morial Convention Center 208

11:15AM Q16.00001 Cell migration through connective tissue in 3-D , BEN FABRY, Department of Physics, University of Erlangen-Nuremberg, Germany — A prerequisite for metastasis formation is the ability of tumor cells to invade and migrate through connective tissue. Four key components endow tumor cells with this ability: secretion of matrix-degrading enzymes, firm but temporary adhesion onto connective tissue fibers, contractile force generation, and rapid remodeling of cytoskeletal structures. Cell adhesion, contraction, and cytoskeletal remodeling are biomechanical parameter that can be measured on single cells using a panel of biophysical methods. We use 2-D and 3-D traction microscopy to measure contractile forces; magnetic tweezer microrheology to estimate adhesion strengths, cytoskeletal stiffness and molecular turn-over rates; and nanoscale particle tracking to measure cytoskeletal remodeling. On a wide range of tumor cell lines we could show that cell invasiveness correlates with increased expression of integrin adhesion receptors, increased contractile force generation, and increased speed of cytoskeletal reorganization. Each of those biomechanical parameters, however, varied considerably between cell lines of similar invasivity, suggesting that tumor cells employ multiple invasion strategies that cannot be unambiguously characterized using a single assay.

11:51AM Q16.00002 Dynamics of active cellular response under stress , RUMI DE, Weizmann Institute of Science, Israel, ASSAF ZEMEL, University of California, Davis., SAMUEL SAFRAN, Weizmann Institute of Science, Israel — Forces exerted by and on adherent cells are important for many physiological processes such as wound healing and tissue formation. In addition, recent experiments have shown that stem cell differentiation is controlled, at least in part, by the elasticity of the surrounding matrix. Using a simple theoretical model that includes the forces due to both the mechanosensitive nature of cells and the elastic response of the matrix, we predict the dynamics of orientation of cells. The model predicts many features observed in measurements of cellular forces and orientation including the increase with time of the forces generated by cells in the absence of applied stress and the consequent decrease of the force in the presence of quasi-static stresses. We also explain the puzzling observation of parallel alignment of cells for static and quasi-static stresses and of nearly perpendicular alignment for dynamically varying stresses. In addition, we predict the response of the cellular orientation to a sinusoidally varying applied stress as a function of frequency. The dependence of the cell orientation angle on the Poisson ratio of the surrounding material can be used to distinguish systems in which cell activity is controlled by stress from those where cell activity is controlled by strain. **Reference:** Nature Physics, vol. 3, pp 655 (2007).

12:03PM Q16.00003 Observation of Non-local Mechanical Responses to Locally Applied Forces in Cells using Magnetic Micropost Arrays , CORINNE LAMB, YAOHUA LIU, DANIEL REICH, Johns Hopkins University, NATHAN SNIADECKI, University of Washington, CHRISTOPHER CHEN, University of Pennsylvania — The process of force transduction by living cells is linked to changes in cellular function. To study the cellular response to applied forces, we have developed a novel force detection device, which can also be used to apply external forces to a cell. Cells are cultured atop an array of micrometer scale elastomeric posts, which act as independent sensors to cellular traction forces. An external force is applied to the adherent surface of the cell via a magnetic torque on a cobalt nanowire embedded in a single post. Results measuring the spatially resolved forces exerted by the cell over time indicate two responses: a sudden or a gradual global relaxation of the cell in response to a single force actuation. [1] In both cases, the subcellular distribution of loss in traction forces was not concentrated near the point of stimulation but occurred instead at discrete locations around the cell's periphery. Observation of these adaptive non-local responses is potentially important in understanding how external forces are transduced into biochemical regulators of cell function.

[1]N. Sniadecki, et. al, "Magnetic microposts as an approach to apply forces to living cells," *Proc Natl Acad Sci*, 104, no. 37 (2007): 14553

12:15PM Q16.00004 Substrate Stiffness Detection by Cellular Stress and Strain , SHANG-YOU TEE, PAUL JANMEY, University of Pennsylvania — Cells can detect the stiffness of their microenvironment and use this elasticity information to perform cellular functions. We grow cells in hydrogels of different stiffnesses. We embed particles in the hydrogels and measure the traction forces exerted on the hydrogel by tracking particle motions. We correlate these motions to protein dynamics and deduce the stress-strain relationship that cells use to measure elasticity.

12:27PM Q16.00005 Probing Eukaryotic Chemotaxis with Optically Manipulated Biomimetic Microparticles. , HOLGER KRESS, CECILE MEJEAN, JIN GYU PARK, TAREK FAHMY, ERIC DUFRESNE, Yale University — Chemotactic cells are able to sense chemical gradients and to move towards the source of a chemical agent. Eukaryotic chemotaxis is an important part of the mammalian immune system and poses many questions about the cell's physical mechanisms to detect, process and respond to external stimuli. While an understanding of this process is emerging, new methods for precise, controlled and flexible quantitative cell stimulation are needed to test existing hypotheses. We present such a method which is based on optically manipulated biomimetic microparticles. We are developing colloidal particles that provide controlled release of a chemoattractant. These micro-sources of stimulating agents are positioned with optical tweezers at arbitrary locations close to chemotactic cells in order to apply flexible spatio-temporal stimulation patterns to the cells. We show that chemotactic cell response - directed cell polarization, motility and turning - can be induced by our novel stimulation method. In conjunction with live cell microscopy this method is suitable to study the dynamics of intracellular signaling loops.

12:39PM Q16.00006 Quantifying *Dictyostelium discoideum* Aggregation , COLIN MCCANN, University of Maryland, PAUL KRIEBEL, CAROLE PARENT, National Institutes of Health, WOLFGANG LOSERT, University of Maryland — Upon nutrient deprivation, the social amoebae *Dictyostelium discoideum* enter a developmental program causing them to aggregate into multicellular organisms. During this process cells sense and secrete chemical signals, often moving in a head-to-tail fashion called a 'stream' as they assemble into larger entities. We measure *Dictyostelium* speed, shape, and directionality, both inside and outside of streams, and develop methods to distinguish group dynamics from behavior of individual cells. We observe an overall increase in speed during aggregation and a decrease in speed fluctuations once a cell joins a stream. Initial results indicate that when cells are in close proximity the trailing cells migrate specifically toward the backs of leading cells.

12:51PM Q16.00007 Cell motility as a persistent random walk , SIMON NORRELYKKE, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany. Department of Molecular Biology, Princeton University, FRANK JULICHER, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — We study the stochastic properties of trajectories of individual keratocytes that move on a solid substrate. The distribution of observed velocities exhibits a characteristic maximum at finite speed and a local minimum at zero velocity. This velocity distribution depends on the averaging time during which velocities are measured. To characterize the stochatsic properties of the system, we determine the correlations between longitudinal and transverse components of the acceleration with the instantaneous velocity. The experimental data can be captured by a simplified physical description of cell locomotion where random forces act on a system of two elastically coupled elements, one of which is driven forward by an active process, dragging the second behind.

1:03PM Q16.00008 Role of receptor patch geometry for cell adhesion in hydrodynamic flow , CHRISTIAN KORN, ULRICH SCHWARZ, University of Heidelberg — Motivated by the physiological and biotechnological importance of cell adhesion under hydrodynamic flow, we theoretically investigate the efficiency of initial binding between a receptor-coated sphere and a ligand-coated wall in linear shear flow. Using a Langevin equation that accounts for both hydrodynamic interactions and Browian motion, we numerically calculate the mean first passage time (MFPT) for receptor-ligand encounter. We study how the MFPT is influenced by flow rate, receptor and ligand coverage, and receptor patch geometry. With increasing shear rate, the MFPT decreases monotonically. Above a threshold value of a few hundreds, binding efficiency is enhanced only weakly upon increasing the number of receptor patches. Increasing the height of the receptor patches increases binding efficiency much more strongly than increasing their lateral size. This strong dependance on out-off-plane geometry explains why white blood cells adhere to the vessel walls through receptor patches localized to the tips of microvilli, and why malaria-infected red blood cells form elevated receptor patches (*knobs*). [1] C. Korn and U. S. Schwarz, *Phys. Rev. Lett.* **97**: 138103, 2006. [2] C. B. Korn and U. S. Schwarz. *J. Chem. Phys.* **126**: 095103, 2007

1:15PM Q16.00009 Dynamic friction measurements on living HeLa cells , MARC-ANTONI GOULET, MARIE-JOSÉE COLBERT, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University — The interaction of cells with various interfaces, and especially man-made surfaces, is an active field of research. In our experiment we use a micropipette to measure both the friction and normal force as a cell slides across a surface. A thin substrate, coated with Poly-L-Lysine is brought into contact with a HeLa cell. The adjustable substrate motion is used to study the response of the cell at various normal forces and speeds. Analysis of the micropipette provides dynamic measurements of both the friction and normal force. With our novel setup we are able to probe the attachment/detachment process of living cells.

1:27PM Q16.00010 AFM method to study mechanics of biological cells with real brushy surface. , IGOR SOKOLOV, SWAMINATHAN IYER[1], RAVI GAIKWAD, VENKATESH SUBBA-RAO[2], CRAIG WOODWORTH, Clarkson University — AFM is particular useful for studying biological systems because it can be used on viable cells directly in physiological media. Most of the time, the deformation curves measured with AFM on cells have typical "two layer" behavior. As we see from confocal fluorescent images of cells, the cell surface is not flat and covered by a brush-like structure. Here we describe a simple two-layer model to decouple the force response of these two "layers", the cell body and brush. In contrast with the existent biological methods, AFM is a highly sensitive technique that can provide precise quantitative data on both lengths and grafting densities of the brush while measured directly on viable cells. Moreover, it allows one to decouple true cell rigidity from the contribution of the brush layer. This novel method can be applied to virtually any kind of cells. Ignoring this layer may result in incorrect values of cell rigidity derived from the AFM measurements. We demonstrate the developed method on the example of cancerous and normal human cervical cells.

[1]Present affiliation: The University of Western Australia

[2]Present affiliation: Wayne State University

1:39PM Q16.00011 Dynamical measurement of the physical properties of single cells , MARIE-JOSEE COLBERT, CECILE FRADIN, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University — The mechanical response of living cells to external forces has attracted the attention of many researchers. We have developed a new tool that takes advantage of an 'L' shaped micropipette to micromanipulate a single cell and put it in contact with an adhesive surface mounted on a translation stage. The spring constant of the micropipette is carefully measured and its deflection is used to apply a calibrated force, and probe the mechanical properties of the cell. As the cell is compressed between the pipette and substrate, dynamical measurements of the elasticity of the cell and the adhesion of the membrane to the substrate are obtained by monitoring the displacement of the micropipette. This technique gives access to real time monitoring of the cell response to a constant applied force, thus exploring the relaxation processes of the cell when subjected to deformation.

1:51PM Q16.00012 Computational modeling of cell-cell adhesion and cell-endothelium peeling , KENG-HWEE CHIAM, RAYMOND QUEK, A*STAR Institute of High Performance Computing — We describe the use of computational modeling to study the behavior of cells adhering to one another as well as to the circulatory endothelium. These cells are subjected to shear stress imposed by the circulatory plasma, and may peel from the endothelium as a result. Cells that peel have a higher chance to enter circulation and hence pose a greater threat in cancer metastasis. We use the immersed interface method to model the cells and solve for its biomechanical response. We quantitatively study the peeling dynamics as a function of the cells' material properties and the surrounding fluid's dynamics. We show how cell peeling from the endothelium is hampered by its adhesive interaction with surrounding cells. In addition, a larger aggregate of cells, such as a tumor embolus, peels more readily from the endothelium than smaller ones. These result may give us insight into the concept of cancer metastatic efficiency.

2:03PM Q16.00013 Implications of Cytoplasmic Streaming for Intracellular Transport and Micro-scale Mixing , JAN-WILLEM VAN DE MEENT, IDAN TUVAL, DAMTP, University of Cambridge, WIM VAN SAARLOOS, Lorentz Institute, Leiden University, RAY GOLDSTEIN, DAMTP, University of Cambridge — Found in many large eukaryotic cells, particularly in plants, cytoplasmic streaming is the circulation of their contents driven by fluid entrainment from organelles carried by molecular motors at the cell periphery. Streaming has frequently been conjectured to aid in transport and mixing of molecular species in the cytoplasm, and, by implication, in cellular homeostasis, yet no mechanism quantifying this enhancement has been demonstrated. We solve the flow and its associated advection-diffusion equations for the archetypal 'rotational streaming' found in Characean algae, where the cytoplasm streams up and down along helical bands on the surface of cylindrical *internodal* cells. We find that the spiralling flow induces a secondary circulation, reminiscent of Dean vortices found at higher Reynolds numbers, which leads to the formation of a high-flux boundary layer allowing faster uptake and response to changes in external concentration. This effect constitutes a novel example of how high Peclét number flows can facilitate diffusive transport and mixing at the micro-scale.

Wednesday, March 12, 2008 2:30PM - 5:30PM –

Session S8 DFD: Colloidal Rheology Morial Convention Center RO6

2:30PM S8.00001 Shear Thickening, Gel Elasticity and Internal Stresses in a Colloidal System with Attractive Interactions , CHINEDUM OSUJI, Yale University, DAVID WEITZ, Harvard University — Dilute dispersions of carbon particles in hydrocarbon fluids flocculate, forming colloidal gels with typical fractal scaling of shear modulus with particle volume fraction. Surprisingly, these systems exhibit shear thickening in two regimes. At low shear rates, shear thickening is concurrent with the formation of vorticity-aligned structures, a general phenomenon in attractively-interacting complex fluids, but not previously implicated in shear thickening. At high Péclet numbers, thickening involves degradation of particle clusters and an increase in effective volume fraction. This contrasts with the hard-sphere case where thickening is due to pseudo-jamming events that occur with the growth of hydro-clusters with persistent contacts. On cessation of high shear rate flow, these shear thickened gels display a power-law dependence of elasticity on pre-shear stress and the data can be re-scaled simply to provide a universal response for different particle volume fractions. We propose a mechanism and scaling argument that accounts for this behavior in terms of the stress dependence of the cluster number density during pre-shear. We characterize the internal stresses that result from a shear rate quench from the fluid to the gel state and find that the modulus is directly proportional to the internal stress in the system. At short times, t$\approx 10^3$s, the internal stress decays with a weak power law dependence on time.

2:42PM S8.00002 Microscopic Details of Plastically Sheared Colloidal Gels , GARY L. HUNTER, TIFFANY SOO, DENIS SEMWOGERERE, ERIC R. WEEKS, Emory University — We use fast confocal microscopy to study effects of different shear rates on colloidal depletion gels. Our samples consist of PMMA spheres in a refractive index matched solvent, with polymer added to produce a depletion interaction. We subject these samples to different rates of oscillatory shear with similar strain amplitudes. By tracking the three-dimensional trajectories of several thousand particles, we directly observe how shear modifies the gel's structure at the particle-level and how differences in local structure affect shear-induced dynamics. We find that increasing shear rate significantly increases the rate of plastic bond rearrangement, but that large clusters remain mostly intact, even when the observed deformations are highly non-affine.

2:54PM S8.00003 Delayed Collapse of Colloidal Gels , JUAN-JOSE LIETOR-SANTOS, CHANJOONG KIM, ALBERTO FERNANDEZ-NIEVES, DAVID A. WEITZ, SEAS, Harvard University — We study the behavior of colloidal gels under gravitational forces using a system of polystyrene beads and non-adsorbing polymer to induce depletion attraction between particles. As the interaction energy or the volume fraction decreases, a delayed collapse regime is observed, where the sedimentation of the gels starts with a slow initial compression followed, after a delay time, by a rapid collapse characterized by the coarsening of the structure. By means of changing the density mismatch between the network and the surrounding solvent, we are able to explore the dependence of the delay time and coarsening behavior with the gravitational stress. The results clearly show that, even though only the weakest gels undergo delayed collapse, the gravitational stress is not the trigger leading to the coarsening of the structure, although it certainly affects the time it takes the gel to completely sediment.

3:06PM S8.00004 Effect of Nanoparticle Shape and Size on Shear Rheology , MATT K. PETERSEN, J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories, Albuquerque NM — The effect of nanoparticle shape and size on the shear rheology of nanoparticle suspensions was explored through non-equilibrium molecular dynamics simulations. Composite nanoparticles consisting of rigid Lennard-Jones particles in a Lennard-Jones explicit solvent were modeled using the Müller-Plathe "reverse" perturbation method. A series of suspensions were modeled wherein the nanoparticle volume fraction was held constant while the shape and size of the nanoparticles were varied. Specifically, results for the shear viscosity of spherical, plate, and rod-like nanoparticles of size varying from tens to hundreds of interaction sites will be presented. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

3:18PM S8.00005 Shear Thinning in Nanoparticle Suspensions , PIETER J. IN 'T VELD, MATT K. PETERSEN, GARY S. GREST, Sandia National Laboratories, Albuquerque, NM — Results of large scale non-equilibrium molecular dynamics (NEMD) simulations are presented for nanoparticles in an explicit solvent. The nanoparticles are modeled as a uniform distribution of Lennard-Jones particles, while the solvent is represented by standard Lennard-Jones particles. Here we present results for the shear rheology of spherical nanoparticles of size 5 to 20 times that of the solvent for a range of nanoparticle volume fractions and interactions. Results from NEMD simulations suggest that for strongly interacting nanoparticle that form a colloidal gel, the shear rheology of the suspension depends only weakly on the size of the nanoparticle, even for nanoparticles as small as 5 times that of the solvent. However for hard sphere-like colloids the size of the nanoparticles strongly affects the shear rheology. The shear rheology for dumbbell nanoparticles made of two fused spheres is also compared to spherical nanoparticles and found to be similar except at very high volume fractions. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04- 94AL85000.

3:30PM S8.00006 Viscosity of confined suspensions. , PHILIPPE PEYLA, YOHANN DAVIT, CLAUDE VERDIER, Universite Joseph Fourier - Grenoble, LSP - CNRS - DYFCOM TEAM — In this work, we study experimentally and numerically the viscosity of non-brownian confined suspensions of hard spherical particles confined between two walls in a shear flow. By varying the wall-to-wall distance (gap), we show that the viscosity presents a remarkable behavior as a function of the confinement. A transition occurs from a 3D configuration (no confinement) to a quasi2D (Q2D) one when the wall-to-wall distance becomes smaller than twice the spheres diameter. We find, as expected, that the effective viscosity increases when the gap decreases. This is due to dissipation which is enhanced for smaller gaps. But, more precisely, when the wall-to-wall distance decreases, the linear term in volumic fraction (diluted case) increases while the quadratic term decreases to zero when the suspension reaches a Q2D regime and becomes negative for smaller gaps. In a Q2D suspension, it is proven that an anti-drag effect holds between two particles which move perpendicularly to their connecting line. Experimental measurements on diffusion coefficients have been achieved for colloidal Q2D suspensions by Cui et al [1] which shows this behavior without any ambiguity. We suspect that such anti-drag interactions can affect the viscosity of Q2D semi-diluted suspensions. [1] B. Cui, H. Diamant, B. Lin and S. Rice, Phys. Rev. Lett., vol. 92, 258301 (2004)

3:42PM S8.00007 Rate dependence, drag balance and role of disorder in linearly sheared foams. , GIJS KATGERT, MATTHIAS E. MÖBIUS, MARTIN VAN HECKE, Kamerlingh Onnes Laboratory, Leiden University — We linearly shear a bidisperse foam monolayer sandwiched between a glass plate and a fluid surface over 3 orders of magnitude in driving velocity. We find strongly rate-dependent velocity profiles, which become increasingly shear banded with shear rate. We also confirm previous findings that monodisperse foam layers exhibit rate-$independent$ velocity profiles. Both behaviors are quantitatively captured in a model that balances the viscous drag forces in the foam, provided that we assume the average drag force between bubbles in disordered foams to scale differently than the drag force at the bubble scale. We confirm the scaling of the drag forces in both mono- and bidisperse foams by independent rheological measurements, and confirm the crucial role of disorder on the flow of foams.

3:54PM S8.00008 Shear Modulus of a Depletion-Induced Colloidal Gel , CHANJOONG KIM, DAVID A. WEITZ, Department of Physics and HEAS, Harvard University — Mechanical properties of a colloidal gel are of great interest because they are related to the processability of the colloidal dispersion and its stability. We measure the shear modulus for colloidal gel networks induced by depletion attraction and determine the relationship between the strength of the depletion attraction and the magnitude of the shear modulus.

4:06PM S8.00009 ABSTRACT WITHDRAWN –

4:18PM S8.00010 Irreversible flow-induced vitrification of nanoemulsions by extreme droplet rupturing , JAMES N. WILKING, Dept. of Chemistry, University of California- Los Angeles, THOMAS G. MASON, Depts. of Physics and Chemistry, University of California- Los Angeles — Some materials weaken through fracturing when subjected to extreme stresses. However, breaking down repulsive bits of condensed matter that are dispersed in a viscous liquid can also potentially cause a dramatic and irreversible increase in the dispersion's elasticity. Here, we demonstrate this principle using dispersions of one liquid in another immiscible liquid. Anionically stabilized microscale emulsions are subjected to a history of extreme high-pressure microfluidic flow, causing the droplets to rupture to nanoscale sizes. As the droplet radius decreases below 100 nm, the nanoemulsion can develop an unusually large elastic modulus, even at droplet volume fractions far below maximal random jamming of uniform hard spheres. Thus, through the history of applied flow, a liquid microscale emulsion can be transformed and vitrified into an elastic nanoemulsion of disordered repulsive droplets without altering the composition. Furthermore, we show that systematic macroscopic shear rheology of the nanoemulsion glass as a function of the droplet volume fraction can be effectively used as a surfaces forces apparatus to deduce the screened Debye interaction potential as a function of separation between the droplet interfaces.

4:30PM S8.00011 Hindered rising in aggregating polydisperse particle suspensions , SHIHAI FENG, KIM RASMUSSEN, ALAN GRAHAM, BING DAI, Los Alamos National Lab — We describe a direct simulation method that effectively determines the appropriate hindered rising behavior of polydisperse particle suspensions. Our method allows adequate representation of the hydrodynamic interactions as well as system specific colloidal interactions. Simulation results are in good agreement with experimental data obtained by MRI imaging. Our results demonstrate the importance of particle aggregation in the hindered rising suspensions.

4:42PM S8.00012 Self-organized criticality of slowly sedimenting sheared suspensions , WEINING MAN, LAURENT CORTE, Physics Department, New York University, SHARON GERBODE, Department of Physics, Cornell University, DAVID PINE, PAUL CHAIKIN, Physics Department, New York University — Suspensions of neutrally buoyant particles driven by slow periodic shear can undergo a dynamical phase transition from an absorbing reversible steady state to a fluctuating irreversible state. For a given strain amplitude γ, this transition occurs at a specific critical volume fraction Φ_c. However, if the particles are not neutrally buoyant, they either sink to the bottom or float to the top of the container. New experiments and simulations show that under periodic shear, the particles resuspend, however, and that for a given strain amplitude γ, the particles evolve towards the critical concentration Φ_c without any external intervention. In that case, particle collisions nucleated at the bottom of the shear cell propagate through the sample and keep the system suspended close to the critical volume fraction $\Phi_c(\gamma)$. Hence, slowly sedimenting particles under oscillatory shear appear as a new class of self-organized critical systems hitherto unreported.

4:54PM S8.00013 Random organization: A dynamical phase transition , LAURENT CORTE, DAVID J. PINE, PAUL M. CHAIKIN, Center for Soft Matter Research, NYU — We introduce a simple model motivated by recent experiments in sheared suspensions. We show that completely random displacements of colliding particles are sufficient to generate an organized state where further collisions are suppressed. This organization by self-activated random walkers presents a much more efficient process than when all particles are diffusing. It only occurs provided that the density in particle is lower than a critical value ρ_c and is characterized by a dynamical phase transition. A mean-field description captures the existence of this transition. It suggests that the value of ρ_c is determined by the ratio p_s/p_c, where p_s is the probability for a pair of colliding particles to separate and p_c is the probability that a "quiet" particle be collided. Our results also reveal that the ordering can be enhanced by straining the system periodically. However, these more organized states become less and less accessible as the strain amplitude is increased.

5:06PM S8.00014 X-ray photon correlation spectroscopy in a shear flow , ANDREI FLUERASU, European Synchrotron Radiation Facility — X-ray photon correlation spectroscopy was used to measure the diffusive dynamics of colloidal suspensions in a shear flow. The results presented here show how the intensity autocorrelation functions measure a coupling between the diffusive dynamics of the particles and their flow-induced, convective motion. However, in the limit of low flow/shear rates, it is possible to obtain the diffusive component of the dynamics. The conditions under which this is possible are easier to achieve at higher values of the scattering wavevector q and this may provide an advantage of X-ray over, for e.g. light, photon correlation spectroscopy. In recent work (A. Fluerasu et al., submitted, 2007) we have shown this result to hold for dillute (particle volume fraction $\Phi \approx 10$ %) suspensions when the correlation functions probe, basically, the self-diffusion of individual, non-interacting particles. Here we will also adress the collective motion of concentrated suspensions of hard-sphere systems (Φ up to 50 %) and study the coupling between the shear-induced response and the collective diffusion of the suspension. An important benefit of this experimental strategy over more traditional X-ray methods, is the minimization of X-ray induced beam damage, which makes the method suitable for the study of the dynamical properties of a large class of complex soft-matter and biological fluids.

5:18PM S8.00015 Electrophoretic "Equilibrium" Profile of Charged Colloids , ROMAIN PLANQUES, PAUL CHAIKIN, Dept. of Physics, New York University — We perform an electrophoresis experiment of a concentrated colloid against a semipermeable membrane. The electric field forces the charged particles against the membrane and sets up a concentration profile similar to that of a colloid in gravitational sedimentation equilibrium where gravitational forces compete against the osmotic pressure gradient. In the present case there is a current which flows through the electrolyte so the system reaches a steady state profile rather than equilibrium. The electric field, colloid and ionic concentrations adjust self consistently to produce the profile. We use 91 nm polystyrene spheres with sufficient charge that they crystallize and observe their Bragg scattering as a function of height to determine the lattice spacing and particle concentration. We also use 700nm spheres and obtain their concentration profile with X-ray absorption. The fluid flow is zero for a capped system. Connecting a return tube from the supernatant side above the electrophoretic sediment to below the filter yields an electroosmotic flow and circulation. The profile changes substantially and allows us to study the hydrodynamic interactions as a function of concentration for the electrophoresing particles.

Thursday, March 13, 2008 8:00AM - 10:24AM –

Session U8 DFD: Colloidal Manipulation Techniques Morial Convention Center RO6

8:00AM U8.00001 Local perturbation caused by a particle driven through a 2-D colloidal suspension , CARA HAGEMAN, VIKRAM PRASAD, ERIC R. WEEKS, Emory University — When polystyrene colloids are placed at a decane-water interface they form different phases based on their area fraction. These phases are: liquid, liquid-hexatic, hexatic and crystalline. In particular, the hexatic-crystal transition is characterized by a change in the functional form of the correlation functions and the density of defects. We study this system for area fractions near the hexatic-crystal transition. Using a laser tweezer we trap and drag a particle along the interface and observe its effect on the surrounding colloids. We observe a change in the local density of defects and a decay in the perturbed motion of colloids away from the trapped particle, revealing a length scale. We measure this length scale as a function of area fraction of the colloids and the applied velocity of the trapped particle.

8:12AM U8.00002 Microrheology of a sticking transition , SHOBO BHATTACHARYA, PRERNA SHARMA, SHANKAR GHOSH, Tata Institute of Fundamental Research, Mumbai, India 400005 — The phenomenon of colloidal deposition in presence of shear is studied by using an optical tweezer to hold a colloidal particle in close proximity of a plate subject to a sinusoidal in-plane shaking. Through the measurement of the real and imaginary parts of the particle's response function, the coupling between the particle and the plate is found to evolve from a viscous regime to an elastic regime through an intermediate regime of time-dependent enhancement of viscoelasticity, reminiscent of aging in glasses. The sticking transition can be described in a scenario of hindered Stokes-Einstien diffusion and the Maxwell model of viscoelasticity. Upon changing the bead -plate interaction or the strength of the drive, three regimes of response: stick, stick-slip and slip are observed. The observed behavior has analogies to jamming in granular materials and the glass transition in viscous liquids.

8:24AM U8.00003 A New Diffusion NMR Experimental Model System for Studies of Bidisperse Colloids[1] , ANAND YETHIRAJ, SWOMITRA PALIT, Department of Physics and Physical Oceanography, Memorial University of Newfoundland — A method to prepare monodisperse colloidal particles that are simultaneously NMR-visible and fluorescent is described. A systematic approach to obtain spectrally resolved diffusion coefficients for every component (colloid and solvent) in a monodisperse colloidal suspension is presented. We also prepared bidisperse colloidal suspensions where each colloid component has a distinct NMR spectral signature, and obtained the diffusion coefficient of both colloid species and solvent simultaneously, in concentrated colloidal suspensions with volume fractions between 20 and 50 %. This colloidal model system enables the study of bidisperse colloids at different size ratios and number ratios.

[1]This work is supported by NSERC (Canada).

8:36AM U8.00004 Universal exponential tails in the displacement distribution observed in an attractive colloidal glass , YONGXIANG GAO, MARIA KILFOIL, McGill University — Dynamical heterogeneities exist ubiquitously in glassy materials. They manifest themselves as a non-Gaussian distribution of the constituent particle displacements, that is, the self part of the van Hove correlation function. Though the shape of the tail of the distribution looks exponential or nearly exponential, not until recently has serious attention been paid to it. We observe pure exponential behavior—neither stretched nor compressed—over a wide range of volume fractions and time scales in an attractive colloidal system on the route to attractive glass transition. We observe universal behavior as all the distributions over a wide range of τ and ϕ can be scaled together. The tails arise from the mobile sub-component of the constituent particles. If time permits, I will also show our studies on the structure of colloidal gels and attractive glasses in terms of a translational order parameter and an orientational order parameter, under different interaction strength, volume fraction and buoyancy matching conditions.

8:48AM U8.00005 Point response of a 2D packing of soft colloidal spheres near the jamming transition.[1] , PETER J. YUNKER, DANIEL T. N. CHEN, ZEXIN ZHANG, ARJUN G. YODH, University of Pennsylvania — We have created a 2D jammed packing by confining a bidisperse mixture of thermoresponsive NIPA microgel spheres between two glass slides with a thickness of roughly the larger sphere diameter. The packing is subjected to a point compression created by local heating with optical tweezers. We use particle tracking microscopy to characterize the response as a function of particle volume fraction both above and below the jamming transition.

[1]This work was support by MRSEC grant DMR-0520020 and NSF grant DMR-0505048.

9:00AM U8.00006 Local perturbations of dense colloidal suspensions , GIANGUIDO C. CIANCI, ERIC R. WEEKS, Department of Physics, Emory University — A rapid temperature quench can transform a liquid into a disordered solid: a glass. We model glassy materials using dense colloidal suspensions, where the transition is induced by increasing the number density rather than decreasing temperature. This transition has drawn significant attention because it poses numerous fundamental questions. For example, close to the glass transition temperature a small decrease in temperature can cause the viscosity of the liquid to increase by 14 orders of magnitude. Meanwhile the structure remains essentially unchanged — there is no growing static length scale accompanying the transition. Fast laser scanning confocal microscopy allows us to directly observe and track thousands of colloidal particles in real time. We add a small number of superparamagnetic colloids in the sample and pull them with an external magnet. The motion of a magnetic probe locally perturbs the dense suspension and highlights its heterogeneous structure. We examine the dependence of the affected region's size on density and applied magnetic force.

9:12AM U8.00007 Understanding the dynamics of closely packed microgel particles , MELAKU MULUNEH, HANS WYSS, GIOVANNI ROMEO, JOHAN MATTSSON, ALBERTO FERNANDEZ-NIEVES, JINWOONG KIM, DAVID WEITZ, Harvard University, WEITZ COLLABORATION — Soft particles such as microgel suspensions have important applications in industry, which exploit their unusual structural and rhelogical properties. Despite their relevance, the fundamental physics that controls their behavior remains poorly understood. Intriguingly, microgels act as fluid even at high density. Techniques such as rheology, microscopy, and light scattering have been used to probe the macroscopic properties of these materials – however, the underlying physical mechanisms demand further investigation. We use confocal microscopy to image the local dynamics of highly packed microgels. The gel particles are tracked over time to obtain information about the short and long range correlations of the local particle motion. We probe their response to changes in environmental factors such as temperature or pH using light scattering. The results obtained not only help us understand the origins of the observed macroscopic behavior, but also give us information on the dynamics of glassy arrest in general.

9:24AM U8.00008 Colloidal Particle Geometry and Its Effect on Optical Trapping , RACHAEL HARPER, ALEX LEVINE, Department of Chemistry & Biochemistry, University of California Los Angeles — Recent experiments by Wilking and Mason (Europhysics Letters, in press) on the laser trapping of colloids of various shapes (the letters of the alphabet) show that for identical chemistries the trapping force varies wildly with particle shape. In fact, certain shapes do not trap at all. Motivated by these experimental results, we explore the trapping of particle of variable shape using a ray-optics simulation. This numerical tool allows us to perform Monte Carlo integrations of the total trapping forces and torques for a series of objects such as a cross (the letter "x") or a beam (the letter "I"). We find that certain shapes feature bi-stable trapping positions/orientations, and some, indeed, do not allow for trapping at all.

9:36AM U8.00009 Modeling pore formation in lipid membranes via Janus nanoparticles , ALEXANDER ALEXEEV, Georgia Institute of Technology, WILLIAM E. USPAL, MIT, ANNA C. BALAZS, University of Pittsburgh — Phospholipid membranes, which separate the cytoplasm from the extracellular environment in biological cells, embed a large diversity of proteins. Some proteins form pores for the free transport of small molecules and ions across the membrane. Here, we use coarse grained numerical simulations to design a synthetic membrane, where pores can be formed "on demand." Specifically, we use dissipative particle dynamics to probe the interaction between bilayer membranes and nanoparticles. The particles are nanoscopic Janus beads that comprise both hydrophobic and hydrophilic portions. We demonstrate that when the membrane is ruptured due to an external stress, these nanoparticles diffuse to the free edge of the membrane and form stable pores, which persist after the stress is released. Pore size depends on the architecture and concentration of the nanoparticles. Once a pore is formed, a small increase in membrane tension readily reopens the pore allowing rapid transport through the membrane.

9:48AM U8.00010 Three Dimensional Rotational Motion of Colloidal Clusters , JUSTIN CARAM, Harvard University, Department of Chemistry and Chemical Biology, VINOTHAN MANOHARAN, Harvard University, Department of Physics and School of Engineering and Applied Sciences — We will present the results of a study into the three dimensional rotational and translational diffusion of colloidal clusters, especially dimers and trimers. We will have accomplished this study using both diffraction pattern and holograph analysis, as well as depolarized dynamic light scattering. We believe that trimers break into discrete rotational diffusion constants dependent on their geometries. These findings can be matched to the results for the rotational decay in the correlation function generated by DDLS. Understanding these diffusion constants is important to the understanding of protein and liquid crystal dynamics in solution. Furthermore, developing depolarized dynamic light scattering experimental strategy for non ellipsoidal systems may help to determine 3-dimensional hydrodynamic extent of such systems in solution.

10:00AM U8.00011 Anomalous Rotation of a Pair of Spherical Particles in AC Electric Fields , PUSHKAR LELE, ERIC FURST, University of Delaware — Suspensions of colloidal particles are observed to form angled bands and vortices near surfaces in AC electric fields. We map the critical frequencies and field biases at which particles phase separate in to bands and the vortices gradually set in. The results from such mapping experiments are interpreted based on measurements of anomalous rotation on a pair of colloidal particles held in blinking optical tweezers. Our observations suggest that particle pair rotation is the characteristic motion in vortices and that the polarization of double layer around the particles influences the angular velocity of the vortex revolution. Increasing the electrolyte concentration of the medium or the frequency of the electric field results in reduction of the rotation. Based on these results, the suspension behavior can be "tuned" by changing the ionic strength, field strength, field frequency and particle size.

10:12AM U8.00012 Interferometric and holographic imaging combined: correlating interface deformations with 3D tracking of interfacial particles , DAVID KAZ, VINOTHAN MANOHARAN, Harvard University — We employ the techniques of digital holography and interference phase mapping to investigate particles on interfaces. Digital holography is used to track the positions of small (micron sized) particles to within a few nanometers in three dimensions, while optical interferometry maps interfacial deformations to within a few tens of nanometers. By utilizing both techniques simultaneously, we correlate the 3D position of particles trapped on an interface with deformations of that interface at up to 1000 frames per second. Such comprehensive data will serve to answer questions regarding the capillary interactions of particles on an interface.

Thursday, March 13, 2008 11:15AM - 2:03PM –

Session V8 DFD: Liquid Crystals I: Structure and Defects Morial Convention Center RO6

11:15AM V8.00001 Effect of Concentration Variations on the Interaction of a Sm-A Liquid Crystal and a Nanoparticle[1] , LUZ J. MARTINEZ-MIRANDA, University of Maryland, College Park, LYNN K. KURIHARA, Navy Research Lab, Washington, DC, RAHINA S. RABIU[2], University of Maryland and Norfolk State University — We have observed the evolution of the interaction between a Sm-A Liquid Crystal (8CB) and a nanoparticle as the concentration of the nanoparticle is reduced from 30% wt to 0.1%wt. We have observed that a linear structure is observed as the concentration of the particle falls below 15% wt. There is a difference between the functionalization compounds as observed in the study of the 30% wt mixtures. In addition, we have observed that the influence of the nanoparticle in the ordering or disordering of the liquid crystal can be quantified through the integrated intensity of the x-ray signal.

[1]We acknowledge NSF-DMR grant number 0520471 for partial support of this work.
[2]REU student

11:27AM V8.00002 Simulating defect structures in nematic liquid crystal shells[1] , LENA LOPATINA, ANDREW KONYA, JONATHAN SELINGER, ROBIN SELINGER, Liquid Crystal Institute, Kent State Univ, ALEX TRAVESSET, Dept of Physics and Astronomy, Iowa State Univ — Recent theoretical and experimental studies have investigated nematic liquid crystals confined to a shell between two spheres. When the shell is very thin, the structure provides an experimental realization of nematic order and defects in a 2D curved geometry. As the shell becomes thicker, the behavior crosses over to a 3D liquid crystal, with different types of defects. To study this dimensional crossover, we perform simulations of nematic order in a shell. For these simulations, we use a disordered lattice, or mesh, constructed through random sequential adsorption on the inner surface, the outer surface, and within the bulk of the shell, with a nematic director on each site of the mesh. By minimizing the energy, we determine the nematic texture as a function of the radii and thickness of the shell, and as a function of the off-center displacement of the inner sphere. The results show a crossover between half-charged vortex line defects for thin shells and boojum pairs for thicker shells, and demonstrate a new equilibrium state with two vortex lines and one boojum pair. They also show a complex evolution of the structures and energy as the inner sphere moves off-center.

[1]Supported by NSF DMR-0605889 and DMR-0426597 and by ICAM.

11:39AM V8.00003 String defects in smectic-C monolayers and hybrid nematic films[1]

FANGFU YE, ZHAO LU[2], LENA LOPATINA, JONATHAN SELINGER, Liquid Crystal Institute, Kent State Univ, ALEX TRAVESSET, Dept of Physics and Astronomy, Iowa State Univ — Defects are important in determining the structure and statistical mechanics of liquid crystals. In this project, we study the structure of topological defects in smectic-C monolayers and hybrid nematic films. When subjected to boundary conditions requiring a total topological charge of +1, the classical xy model in a flat disk geometry has a ground state of a single vortex of charge +1. By comparison, perfect nematics with directors in the same 2D geometry have two +1/2 vortices repelling each other. We show that slightly tilting directors out of the plane to form a smectic-C monolayer yields two +1/2 vortices bound together by a domain wall, which we call a string defect. We also develop a model easily testable in experiments, in which a thick nematic film is constrained in a cell with weak homeotropic anchoring on one surface and strong planar anchoring on the other surface. For this model, we derive the phase diagram and investigate how the length of string defects changes with the thickness of the cell. We further present numerical simulations of the nematic director in the hybrid film.

[1]Supported by NSF DMR-0605889 and DMR-0426597 and by ICAM.
[2]Currently at College of Veterinary Medicine, Cornell Univ.

11:51AM V8.00004 Coherent anti-Stokes Raman scattering polarized microscopy of 3D director structures in liquid crystals[1]

IVAN SMALYUKH, University of Colorado at Boulder, ALEXANDER KACHYNSKI, ANDREY KUZMIN, PARAS PRASAD, The State University of New York at Buffalo — We demonstrate labeling-free three-dimensional imaging of director structures in liquid crystals using coherent anti-Stokes Raman scattering (CARS) polarized microscopy [1]. Spatial mapping of the structures is based on the strong sensitivity of a polarized CARS signal to the orientation of selected chemical bonds of anisotropic molecules in liquid crystals. As an example, we study director structures in cholesteric, nematic, and smectic materials. We demonstrate that the CARS images of molecular orientation patterns are consistent with the structure models and with the respective computer-simulated CARS textures.
[1]. A.V. Kachynski, A.N. Kuzmin, P.N. Prasad, and I.I. Smalyukh, Appl. Phys. Lett. 91, 151905 (2007).

[1]Research was supported by the Directorate of Chemistry and Life Sciences of Air Force Office of Scientific Research, by International Institute for Complex Adaptive Matter, and the National Science Foundation, Grant DMR #0645461.

12:03PM V8.00005 Light Scattering Study of Biaxiality in Nematic Liquid Crystal Tetrapodes

KRISHNA NEUPANE, SHINWOONG KANG, SUNIL SHARMA, D. CARNEY, T. MEYER, GEORGE H. MEHL, DAVID W. ALLENDER, SATYENDRA KUMAR, SAMUEL SPRUNT, Department of Physics, Kent State University — We have performed dynamic light scattering studies on thermotropic liquid crystalline tetrapodes [1], which reportedly exhibit a uniaxial to biaxial nematic phase transition. Our results [2] support the existence of the biaxial nematic phase in tetrapodes. The uni - to biaxial transition is found to be weakly first-order in a 4-ring tetrapode and second-order in a 3-ring tetrapode, while the isotropic to uniaxial nematic transition is weakly first order in both materials. The temperature dependence of the relaxation rates of the biaxial order parameter modes, and of the intensity associated with biaxial director fluctuations, is explained by a Landau-deGennes model of the free energy.
[1] R. Elsasser, J. W. Goodby, G. H. Mehl, D. Rodriguez-Martin, R. M. Richardson, D. J. Photinos, and M. Veith, Mol. Cryst. Liq. Cryst. **402**, 237 (2003)
[2] K. Neupane, S. W. Kang, S. Sharma, D. Carney, T. Meyer, G. H. Mehl, D. W. Allender, S. Kumar, and S. Sprunt, *Phys. Rev. Lett.* **97**, 207802 (2006)

12:15PM V8.00006 Effects of dielectric relaxation on the director dynamics of uniaxial nematic liquid crystals[1]

MINGXIA GU, YE YIN, SERGIJ V. SHIYANOVSKII, OLEG D. LAVRENTOVICH, Chemical Physics Interdisciplinary Program, Liquid Crystal Institute, Kent State University, Kent, Ohio 44242, USA — We derive the reorienting dielectric torque acting on the director, considering the frequency dependence of the dielectric tensor. The model takes account into the effects of multiple relaxations in both parallel and perpendicular components of the dielectric tensor and predicts the "dielectric memory effect" (DME), i.e., dependence of the dielectric torque on both the "present" and "past" values of the electric field and the director. In a sharply rising electric field, the DME slows down director reorientation for the materials whose dielectric anisotropy is positive at low frequencies, but speeds up the response for the dielectrically negative materials. We also demonstrate, both theoretically and experimentally that an induced "memory" polarization leads to a dielectric torque in the switch-off phase which has an opposite sign to that of the LC's dielectric anisotropy, when a specific switching-off profile is used; this reverse torque accelerates the director relaxation back to the equilibrium state.

[1]Supported by DOE Grant No. DE-FG02-06ER 46331.

12:27PM V8.00007 Condensation of lyotropic chromonic liquid crystals by additives[1]

LUANA TORTORA, H.-S. PARK, Liquid Crystal Institute, Kent State University, Kent, OH 44242, S.-W. KANG, Department of Physics, Kent State University, Kent, OH 44242, S. KUMAR, Department of Physics, Kent State University, Kent, OH 44242 and DMR NSF, K.V. KAZNATCHEEV, Canadian Light Source, SK S7N 0X4, Canada, O.D. LAVRENTOVICH, Liquid Crystal Institute, Kent State University, Kent, OH 44242 — Lyotropic chromonic liquid crystals (LCLCs) are formed by molecules with rigid polyaromatic cores and ionic groups at the periphery that aggregate in water. Condensation of LCLCs can be driven by polyamines, organic salt and neutral polymers. At a suitable concentration of additives, a nematic LCLC demixes into a coexisting isotropic phase and a condensed phase with birefringence higher than that in the original N. By employing synchrotron X-ray scattering we demonstrate the formation of a columnar hexagonal (C) phase. Scanning transmission X-ray microscopy, LC PolScope and fluorescent confocal microscopy allow us to map the relative concentration of components in the condensed and isotropic regions. Both electrostatic and entropy effects contribute to the condensation.

[1]Supported by NSF DMR 0504516, DMR 076290, AFOSR MURI FA9550-06-1-0337, Samsung Electronics Corp.

12:39PM V8.00008 Interactions in the NOBOW and 8CB Mixtures[1]

DONG CHEN, CHENHUI ZHU, NOEL CLARK, Department of Physics, University of Colorado, Boulder — Mixtures of a bent-core mesogen (NOBOW) and a calamitic mesogen (8CB) are studied using X-ray diffraction (XRD), polarized light microscopy and freeze fracture electron microscopy (FFEM). XRD shows that as the 8CB concentration increases, the transition temperature of Iso-B4 decreases and the correlation length of NOBOW B4 decreases while the correlation length of 8CB SmA increases. Polarized light microscopy reveals that the mixtures have larger chiral domains than pure NOBOW and when the phase of 8CB changes to SmA, they show the same boundary as the chiral domains. FFEM images show more details on the structure of the mixtures. Along with the experiments, we will present theoretical studies on the interactions in the NOBOW and 8CB mixtures.

[1]This work is supported by NSF MRSEC Grant DMR-0213918

12:51PM V8.00009 Effect of Solvent Concentration on the Liquid Crystal Phase Transitions of Octylcyanobiphenyl-Hexane Mixtures , KRISHNA SIGDEL, GERMANO IANNACCHIONE, WPI — The effect of a non-mesogenic, low-molecular weight, solvent on the phases of a liquid crystal can be profound. High-resolution ac-calorimetry has been carried out on the isotropic to nematic (*I*-*N*) and the nematic to smectic-*A* (*N*-Sm*A*) phase transitions of the liquid crystal octylcyanobiphenyl (8CB) as a function of hexane concentration. Temperature scans were performed above and below these transition temperatures for all samples. Six 8CB+hexane samples were studied having molar concentrations of 0.017 (0.5% by mass), 0.033 (1%), 0.063 (2%), 0.078 (2.5%), 0.092 (3%) and 0.119 (4%) of hexane. Upon increasing dilution of 8CB by the linear form of hexane, the transition temperatures shift lower while the order of both transitions evolves. These effects may be the consequence of the weakening of the liquid crystal molecular interactions due to the presence of the solvent.

1:03PM V8.00010 Landau potential of polymer stabilized ferroelectric liquid crystals , PAUL ARCHER, INGO DIERKING, The University of Manchester — Polymer stabilized liquid crystals (PSLC) [1] consist of a relatively low concentration of a photo-polymerized monomer (typically less than 10%wt) which is phase separated from the continuous liquid crystal medium. For the case of a polymer stabilized ferroelectric liquid crystal, photo-polymerized in the SmA* phase, the network forms parallel to the smectic layer normal. This results in an elastic coupling between the polymer network and the liquid crystal which alters the characteristics of the SmA* to SmC* phase transition. The generalized model of ferroelectric liquid crystals has been modified to encompass this additional interaction through a polymer coupling coefficient. Analysis of experimental tilt angle and polarization data allows the determination of the polymer coupling coefficient and hence the full Landau potential. Results will be shown and discussed for varying polymer concentration.
[1] I. Dierking, Adv. Mater. **12**, 167 (2000)

1:15PM V8.00011 Varying the optical properties of cholesteric liquid crystals , SABRINA RELAIX, MICHELE MOREIRA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU, MICHEL MITOV, CEMES/CNRS — Cholesteric Liquid Crystals (CLCs) are of particular interest as they form self-assembled photonic band gap (PBG) structures - a macroscopic helical structure, leading to a selective reflection of light - which can be easily tuned by external fields. As PBG materials, CLCs have been used as mirrorless lasers with low lasing thresholds since the density of photon states is suppressed in the reflection band and is enhanced at its edges [1]. The modification of the cholesteric organization – either by the introduction of a pitch gradient across the cell or by the incorporation of nanoparticles in the medium – has direct consequences on the PBG and hence the reflected intensity [2,3]. In this presentation, I will describe the variations in the optical properties of CLC caused by these modifications and will discuss possible applications, such as tuning the CLC laser wavelength or adjusting the laser threshold.
[1] P. Palffy-Muhoray et al., Phil Trans R Soc A 364, 2747 (2006)
[2] S. Relaix et al., Appl. Phys. Lett. 89, 251907 (2006)
[3] S. Relaix et al., Liq. Cryst. 34, 1009 (2007)

1:27PM V8.00012 Three-dimensional imaging of chemical bond orientation in liquid crystals by coherent anti-Stokes Raman scattering microscopy.[1] , OLEG D. LAVRENTOVICH, HEUNG-SHIK PARK, Liquid Crystal Institute and Chemical Physics Program, Kent State University, Kent, OH 44242, BRIAN G. SAAR, X. SUNNEY XIE, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA 02138 — Coherent anti-Stokes Raman scattering (CARS) microscopy is used to provide three-dimensional chemical maps of liquid crystalline (LC) samples without the use of external labels. CARS is a polarization-sensitive optical imaging technique that derives contrast from Raman-active molecular vibrations in the sample. Compared to other three-dimensional imaging techniques, CARS offers the most rapid chemical characterization available without the use of external dyes or contrast agents. Examples that illustrate the applicability of CARS microscopy to LCs include textures and defects in nematic and smectic LC, electric Frederiks transition.

[1]Supported by NSF DMR 0504516, DBI-0649892, Keck Foundation, AFOSR MURI FA9550-06-1-0337

1:39PM V8.00013 Low electric field induced phase transition of the B1 bent-core liquid crystal phase to a switching phase , J. KIRCHHOFF, L.S. HIRST, Florida State University — Liquid crystal materials that have ferroelectric and antiferroelectric phases are useful in applications due to their switching properties. The B1 bent-core liquid crystal phase is a columnar phase that does not exhibit switching. A transition from the B1 liquid crystal phase to a switching phase has been seen at an electric field of 10 V/μm, which is much lower than previously seen fields of greater than 25 V/μm [1]. This transition is irreversible upon reduction of the applied field and switching continues almost threshold-less down to an applied field of 40 mV/μm, which has not been previously reported. Any amount of a chiral rod-like dopant increases the field required to transition from the B1 to the switching phase, and the transition becomes reversible with the mixture relaxing back to the B1 phase after a decrease in the electric field. A small concentration of the rod-like dopant also induces a change from the B1 phase to a new liquid crystal phase. These effects were studied using polarized optical microscopy, calorimetry (DSC), and x-ray measurements.
[1] J. Ortega et. al., Phys. Rev. E, **69**, 011703 (2004)

1:51PM V8.00014 Evidence of Broken Reciprocity in Chiral Liquid Crystals , MICHELE MOREIRA, NITHYA VENKATARAMAN, BAHMAN TAHERI, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU — Reciprocity in light scattering is predicated on bounded scattering media with symmetric and linear permittivity, conductivity and permeability. Due to their anisotropy and chirality, cholesteric liquid crystal form periodic dielectric structures. If the periodicity is comparable to the wavelength of light, these phases are self-assembled photonic band gap structures. There appear in the permittivity odd powers of the wave vector resulting from nonlocality and broken inversion symmetry. Evidence of non-reciprocity has been found in optically active crystals by Bennett [1] and in stacks of cholesteric and nematic liquid crystal cells by Takezoe [2]. We present experimental data showing broken reciprocity in transmittance and reflectance in cholesteric cells with different pitches having overlapping but distinct reflection bands. We explain our results in terms of simple analytic descriptions of material properties and propagating modes.
[1] P.J. Bennett, S. Dhanjal, Yu. P. Svirko and N. I. Zheludev, *Opt. Lett.* **21**, 1955 (1996)
[2] J. Hwang; M.H. Song; B. Park; S. Nishimura; T. Toyooka; J.W. Wu; Y. Takanishi; K. Ishikawa; H. Takezoe, *Nat. Mat.* **4**, 383 (2005).

Thursday, March 13, 2008 11:15AM - 2:15PM –

Session V9 DFD: Computational Methods: Multiscale Modeling Morial Convention Center RO7

11:15AM V9.00001 Step decoration studied with first-principles statistical mechanics , YONGSHENG ZHANG, KARSTEN REUTER, Fritz-Haber-Institut der Max-Planck Gesellschaft — With respect to oxidation catalysis or oxide formation, surface defects like steps, kinks, or vacancies are widely believed to play a decisive role, e.g. in form of active sites or as nucleation centers. Despite this suggested importance, first-principles investigations qualifying this role for gas-phase conditions that are representative of these applications are scarce. This is mostly due to the limitations of electronic-structure calculations in tackling the large system sizes and huge configuration spaces involved. We overcome these limitations with a first-principles statistical mechanics approach coupling density-functional theory (DFT) calculations with grand-canonical Monte Carlo simulations, and apply it to obtain the phase diagram of on-surface O adsorption at a (111) step on a Pd(100) surface. The link between the electronic and mesoscopic techniques is achieved by a lattice-gas Hamiltonian expansion, in which we parameterize the lateral interactions affected by the step from DFT calculations at a Pd(117) vicinal surface, and all remaining lateral interactions from calculations at Pd(100). For a wide range of O gas-phase conditions we find the (111) step to be decorated by a characteristic zig-zag structure. Intriguingly, this structure prevails even up to the elevated temperatures characteristic for catalytic combustion reactions, where only small amounts of disordered oxygen remain at the Pd(100) surface.

11:27AM V9.00002 Non-Adiabatic Transition Path Sampling: Application to a Model Proton-Transfer Reaction , LAURA J. KINNAMAN, Physics, U. of Notre Dame, STEVEN A. CORCELLI, Chemistry & Biochemistry, U. of Notre Dame, KATHIE E. NEWMAN, Physics, U. of Notre Dame — A new algorithmic method is discussed, Non-Adiabatic Path Sampling (NAPS), which combines features of transition path sampling (TPS) and molecular dynamics with quantum transitions (MDQT). The goal is to ultimately address problems which involve excited and coupled electronic states, as well as large systems and long timescales (*e.g.*, semiconductor photocatalysis). TPS focuses specifically on trajectories that take a system from reactants to products, which allows the study of chemical processes that are dominated by rare but important events whose timescales are outside the range of direct simulation. In the MDQT algorithm, the nuclear dynamics of the system do not occur on a single Born-Oppenheimer potential energy surface, but rather may involve non-adiabatic transitions between many coupled electronic states. The NAPS algorithm uses the statistical framework of TPS to analyze MDQT trajectories, using the advantages of each method to get results for otherwise inaccessible systems. The algorithm is tested on a simple model of proton transfer: A quantum-mechanical proton in a double-well quartic potential bi-linearly coupled to a thermal bath of classical harmonic oscillators. Results from the model are compared to numerically exact results available in the literature.

11:39AM V9.00003 First-passage Monte Carlo for materials under irradiation[1] , ALEKSANDAR DONEV, VASILY BULATOV, Lawrence Livermore National Labs — The key challenge in simulations of irradiated materials is that of time scale. Typically, atomistic simulations extend to less than one nanosecond whereas kinetic Monte Carlo (kMC) simulations struggle to reach hours of simulated irradiation. Based on a time-dependent Green's function formalism, our new kMC algorithm extends the simulated time horizon from minutes to tens and hundreds of years while retaining uncompromising accuracy. This presents an exciting opportunity to extrapolate, through accurate numerical simulations, the material behavior observed under the short and violent irradiation exposures used in the accelerated material tests, to the much longer reactor material lifetimes.

[1]This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. (UCRL-ABS-236713).

11:51AM V9.00004 OPAL: A New Multiscale Software Architecture Based on MPI-2 , YUN-WEN CHEN, CHAO CAO, Quantum Theory Project and Department of Physics, University of Florida, MING ZHANG, Quantum Theory Project and Department of Computer and Information Science and Engineering, University of Florida, ERIK DEUMENS, Quantum Theory Project and Department of Chemistry and Department of Physics, University of Florida, HAI-PING CHENG, Quantum Theory Project and Department of Physics, University of Florida — Software integration for multi-scale simulations is a time-consuming process. Common practice is to turn the higher level calculation code (e.g. DFT) into a subroutine of the lower level calculation code (e.g. MD). This method often requires non-trivial effort. To avoid these difficulties, we have developed a software package OPAL, within which a minimal development effort is required to build a working multi-scale environment. We report our effort of integrating DL_POLY and SIESTA codes for hybrid quantum-classical simulations. This work is supported the NSF through ITR-medium (NSF/DMR/ITR-0218957) program. The authors want to thank NERSC, CNMS/ORNL and the University of Florida High Performance Computing Center for providing computational resources and support that have contributed to the research results reported within this paper.

12:03PM V9.00005 MP2 calculations for solid state systems[1] , MARTIJN MARSMAN, GEORG KRESSE, Faculty of Physics, University Vienna, and Center for Computational Materials Science — We present *ab initio* total energy calculations at the level of Hartree-Fock + 2nd-order Møller-Plesset perturbation theory (HF+MP2) for extended systems using periodic boundary conditions and a plane wave basis set. To characterize the accuracy of this level of theory, HF+MP2 lattice constants, bulk moduli, and atomizations energies for several archetypical semiconducting and insulating solid state systems are compared to those from density functional theory calculations and experiment. The HF+MP2 description of van der Waals interactions is illustrated for several noble gas solids. Important computational aspects of HF+MP2 calculations within the plane wave full potential projector-augmented-wave (PAW) formalism, most notably the basis set extrapolation of the MP2 correlation energy, are addressed as well.

[1]Supported by the Austrian Fonds zur Förderung der wissenschaftlichen Forschung (START grant Y218)

12:15PM V9.00006 New approaches to the prediction of thermodynamic stability of crystal structures[1] , JOHANNES VOSS, Materials Research Department, Risoe National Laboratory, DTU; Center for Atomic-Scale Materials Design, Department of Physics, DTU, TEJS VEGGE, Materials Research Department, Risoe National Laboratory, DTU — We present new methods for numerical crystal structure optimization and prediction of structural stability on the basis of density functional theory calculations.[1] Comparison to established approaches to the calculation of lattice free energies differing in numerical complexity and accuracy of the results is provided. We show applications of these methods to complex insulators, semiconductors, and metals, and point out variations of our approaches making them suitable for these different classes of materials. We furthermore briefly outline alternative approaches to the prediction of compound stability avoiding the calculation of free energies. [1] J. Voss and T. Vegge, *to be published* (2007)

[1]We acknowledge financial support by the NABIIT program funded by the Danish Research Councils.

12:27PM V9.00007 Solidifying semiconductor nanocrystals from melts: Molecular dynamics simulations , TIANSHU LI, DAVIDE DONADIO, GIULIA GALLI, Department of Chemistry, University of California, Davis — Understanding the nucleation of semiconductor nanocrystals is of fundamental importance in the field of nanoscience. In this study we employ classical molecular dynamics simulations to explore the crystallization of Si nanocrystals from the melt. We focus on the differences between homogeneous and heterogeneous nucleations, where the heterogeneous case is investigated by simulating a liquid slab. In particular, we use the recently developed forward fluxing method [R.J. Allen, D. Frenkel, and P.R. ten Wolde, JCP 124 024102(2006)] to model the evolution of nucleation processes from melts and to compute nucleation rates. We demonstrate that free surfaces act as catalytic nucleation sites by significantly promoting the formation of solid-like small clusters. The presence of solid-like clusters in proximity of the surfaces is found to occur at temperature higher than those at which solid seed nucleation occurs in bulk liquids, highlighting the important role of heterogeneous nucleation under low under-cooling conditions.

12:39PM V9.00008 Ab-Initio Density Functional Calculation of Interatomic Potentials for Large-scale Atomistic Material Simulations. , G.L. ZHAO, Department of Physics and High Performance Computing Laboratory, Southern University and A&M College, Baton Rouge, Louisiana 70813, S. YANG, Department of Physics, Southern University and A&M College — We propose a new method to calculate interatomic potentials, utilizing an ab-initio density functional formalism. The calculated interatomic potentials can be used for large scale atomistic material simulations and predictions. We benchmark the method for the case of copper. We utilized the ab-initio interatomic potential to calculate various properties of transition metal copper, including the lattice constant, the bulk modulus, thermal expansion coefficient, monovacancy formation energy, and phonon frequencies. The calculated results agree very well with experimental values. We further calculated the properties of BCC Cu, utilizing the interatomic potential derived from the electronic structure calculations of FCC Cu, to demonstrate the predictive capabilities of the interatomic potential. The predicted properties of BCC Cu agree very well with experimental and ab-initio density functional results. Part of the work was performed during the stay of G. L. Zhao at Princeton University. The authors gratefully acknowledge the financial support of the National Science Foundation (Award No. 0508245).

12:51PM V9.00009 A New Look at the Evaluation of Embedded Atom Potential Models.[1] , JAMES N. GLOSLI, KYLE J. CASPERSEN, DAVID F. RICHARDS, ROBERT E. RUDD, FRED H. STREITZ, Lawrence Livermore National Laboratory — The embedded atom method (EAM) potentials have been used extensively since introduced by Daw and Baskes in the mid 1980's due to their simple incorporation of many-body effects that are missed by simple pair potentials. The computational cost of the inclusion of this additional physics has traditionally been a second pass over the pair data. We will report on an implementation of the EAM model within a molecular dynamics algorithm (MD) that does not require this second pass, substantially reducing the computer time and memory required for evaluation of the potential. The second pass is avoided by using a forward extrapolation in time of the density derivative of the embedding function $dF(\rho(t))/d\rho$. The error in this approximation is controllable and consistent with the error introduced by the finite time step numerical integrators used in the MD.

[1] This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

1:03PM V9.00010 Electronic structure from Maximum Entropy optimization: Applications to band energy and electronic force computation[1] , HIRO SHIMOYAMA, PARTHAPRATIM BISWAS, The University of Southern Mississippi — We apply a new entropy optimization scheme to study the electronic density of states for complex disordered materials from a knowledge of spectral moments. We employ the Shannon entropy functional in our work and maximize it subject to the moment constraints to construct the spectral distribution of large Hamiltonian matrix[1]. We illustrate the efficiency and the usefulness of the method by reconstructing a number of exact functions, which are difficult to reproduce by other function reconstruction techniques. The local and global convergence properties of the resulting distribution is studied and the band energy and Fermi level are computed with a high degree of precision. An extension of this method to calculate electronic forces is presented for the purpose of using in large-scale molecular dynamics simulation of materials.

[1]University of Southern Mississipi, Grant No. DE00945

1:15PM V9.00011 Lagrangian Time-Reversible Born-Oppenheimer Molecular Dynamics , ANDERS NIKLASSON, Theoretical Division Los Alamos National Laboratory — A Lagrangian generalization of time-reversible Born-Oppenheimer molecular dynamics [Niklasson et al., Phys. Rev. Lett., vol.97, 123001 (2006)] is proposed. The new formulation enables highly efficient symplectic or geometric integrations of both the nuclear and the electronic degrees of freedom that are stable and energy conserving even under incomplete self-consistency convergence. It is demonstrated how the accuracy is improved by over an order of magnitude compared to previous formulations at the same level of computational cost. The proposed Lagrangian includes extended electronic degrees of freedom as auxiliary dynamical variables in addition to the nuclear coordinates and momenta. While the nuclear degrees of freedom propagate on the Born-Oppenheimer potential energy surface, the extended auxiliary electronic degrees of freedom evolve as a harmonic oscillator centered around the adiabatic propagation of the self-consistent ground state (http://arxiv.org/abs/0711.3466).

1:27PM V9.00012 First-principles calculation combined with multicanonical simulation , YOSHIHIDE YOSHIMOTO, ISSP, University of Tokyo, 5-1-5 Kashiwa-no-ha, Kashiwa, 2778581, Japan — To tackle statistical complexities in condensed matters such as phase transitions of atomic structures with first-principles calculations, Yoshimoto have studied the combination of first-principles calculations and multicanonical methods. By the multicanonical methods, phase space of atomic coordinates can be explored efficiently. Among phase transitions, Yoshimoto focused crystal↔liquid transition because it is a basic procedure for material synthesis and formation of objects (casting). The talk will present his recent results : a direct (not a coexisting) simulation of the crystal↔liquid transition by a kind of two-component multicanonical ensemble, a *multi-order multi-thermal ensemble*, with an order parameter defined with structure factors that characterize the transition, and optimization of a model interatomic potential in terms of the ensemble from an accurate one called *thermodynamic downfolding* of a potential. These provide a principle to project a first-principles approach on a model-based approach conserving thermodynamic properties of multiple phases to a maximum extent. The talk will cover the successful applications of the method to the transition of Si and MgO. Ref: Y. Yoshimoto, J. Chem. Phys. 125, 184103 (2006)

1:39PM V9.00013 Topological Properties of Microstructures in Nanocrystalline Materials. , TAO XU, MO LI, Georgia Institute of Technology — Recent experiments show that the topological properties of microstructures in nanocrystalline materials play an important role in the mechanical properties of nanocrystalline materials. However, the fundamental structure-property relationship has not been fully understood due to the difficulties in determining and controlling the microscopic properties of nanocrystalline materials experimentally. In this study, we investigate how different topological properties affect the thermal and mechanical responses of nanocrystalline materials, including grain size distribution, surface area distribution, triple junction length distribution, grain boundary misorientation, etc. Digital microstructures with desired topological properties are generated using Inverse Monte Carlo method and are then relaxed and deformed by large-scale molecular dynamic simulation. In order to characterize the relaxed and deformed digital samples, we use a new grain boundary characterization method to accurately determine the position and thickness of each grain boundary during both relaxation and deformation. Finally, this newly developed algorithm enables us to study the correlation between topological and mechanical properties of nanocrystalline materials.

1:51PM V9.00014 XML Tools for First-Principles Molecular Dynamics Simulations[1] , FRANCOIS GYGI, University of California Davis — We present a set of XML Schema specifications for the representation of electronic structure data and first-principles molecular dynamics (FPMD) simulation data. The schemas (available at http://www.quantum-simulation.org) include the description of FPMD simulation samples and pseudopotentials in an extensible and code-neutral way. Automatic validation of simulation samples can be achieved using publicly available XML parsers such as Apache Xerces-C. We present examples of web-based remote collaboration in which simulation samples and pseudopotentials are accessed using the http protocol. Data analysis using XSLT scripts and a visualization program for remote inspection of simulation samples will also be demonstrated.

[1]Supported by NSF OCI PetaApps program ITR-HECURA 0749217

2:03PM V9.00015 Approximating Densities of States with Gaps using Maximally Broken Time-Reversal Symmetry[1] , ROGER HAYDOCK, C.M.M. NEX, University of Oregon — When a finite cluster of atoms is used to approximate the electronic structure of a macroscopic system, the appropriate boundary condition for electronic states on the surface of the cluster is maximal flow of probability current through the boundary, or maximal breaking of time-reversal symmetry for the states. For continued fraction representations of electronic Greenians, this boundary condition gives excellent results for both the first and second sheets when there is a single band of states. In this work, the approximation is extended to Greenians for multiple bands separated by gaps, such as arise in semiconductors.

[1]Supported by the Richmond F. Snyder Fund

Thursday, March 13, 2008 2:30PM - 5:18PM –

Session W8 DFD: Liquid Crystals II: Dynamics and Topology Morial Convention Center RO6

2:30PM W8.00001 Finite element studies of the soft elastic response in liquid crystal elastomers[1] , BADEL MBANGA, JONATHAN SELINGER, ROBIN SELINGER, Liquid Crystal Institute, Kent State Univ. — When a liquid crystal elastomer film is stretched in a direction transverse to the nematic director, the resulting stress-strain curve typically displays a plateau region, showing a characteristic soft elastic response. Using 3-d nonlinear finite element simulation, we model the formation of orientational domains controlling this mechanical behavior. We investigate the force-displacement response as a function of strain rate, and explore geometric frustration arising from boundary conditions imposed by clamps. We also model mechanical response of polydomain films aligned under external strain. Our 3-d finite element algorithm is based on a Hamiltonian with terms representing elastic potential energy, kinetic energy, and coupling between elastic strain and nematic order. We assume that orientational order of the material relaxes quickly and remains in local quasistatic equilibrium with the instantaneous local strain. Internal dissipation is also included. We intend through this model to further our understanding of the basic physics governing the dynamic mechanical response of nematic elastomers and also provide a useful computational tool for design and testing of potential engineering device applications.

[1]Supported by NSF DMR-0605889.

2:42PM W8.00002 Fluctuating hydrodynamics of nematics for models of liquid-crystal based biosensors via lattice Boltzmann simulations , ORLANDO GUZMAN, JOSE ANTONIO VELEZ, DAVID CASTAÑEDA, UAM-Iztapalapa — Experimental biosensors based on liquid crystals (LC) use nematics to detect the presence of specific analytes, via the optical textures exhibited by the LC at long times. Efforts to model the time evolution of these textures have relied on relaxational models, ignoring transport phenomena. In this work we include hydrodynamics into a model for these LC biosensors, using lattice Boltzmann (LB) methods and assess the effect on the lifetime of multidomain structures, characteristic of high concentrations of analyte. We apply Yeoman's et al. LB algorithm, which reproduces the hydrodynamic equations developed by Beris and Edwards for LCs. We also take into account thermal fluctuations, by adding random perturbations to the hydrodynamic modes. Following Adhikari et al., their amplitude is determined by the Fluctuation-Dissipation theorem and we excite both hydrodynamic and the sub-hydrodynamic modes (also called ghost modes). As a result, we analyze the influence of the fluctuations and hydrodynamics on the movement of topological defects.

2:54PM W8.00003 Viscous properties of bent core nematic liquid crystals measured using a nanoliter viscometer[1] , CHRISTOPHER BAILEY, JOHN HARDEN, ANTAL JAKLI, Kent State University — Since the development of bent core liquid crystal mesogens showing the nematic phase, much work has been done to study the physical properties of these materials in the form of dielectric spectroscopy, dynamic light scattering, and magnetic field induced phase transitions. Some results of these studies showed interesting behaviors such as slow biaxial fluctuations and the possibility of long range tetrahedratic ordering above the nematic phase. Here we report rheological and optical studies on several bent core mesogens in their isotropic and nematic phases. For the rheological studies, we built a viscometer capable of measuring viscoelastic properties with two centipoise resolution with only using 10nL of fluid. Results show abnormal viscosity and optical behavior near the isotropic to nematic phase transition.

[1]Acknowledge: Funding provided by NSF-DMR 0606160

3:06PM W8.00004 Electrically induced twist in smectic liquid-crystalline elastomers[1] , JONATHAN SELINGER, ROBIN SELINGER, Liquid Crystal Institute, Kent State Univ, CHRISTOPHER SPILLMANN, JAWAD NACIRI, B. R. RATNA, Ctr for Bio/Molecular Science and Engineering, Naval Research Lab — Liquid-crystalline elastomers are cross-linked polymer networks covalently bonded to liquid-crystalline units, so that any change in the orientational order influences the shape of the polymer network. As a new approach to developing electrically controllable actuators, we prepare elastomers of chiral smectic-A liquid crystals, which have an electroclinic effect, i.e. a molecular tilt induced by an applied electric field. For thin films in a bookshelf orientation, one would expect the electroclinic effect to cause an in-plane shear of the elastomer, leading to a distortion from a rectangle to a parallelogram. Surprisingly, our experiments find instead that an electric field causes a twisting of the film out of the plane, leading to a helically curved shape. The twist is rapid and reversible, with a helical sense that depends on the sign of the applied field. To explain this electrically induced twist, we develop a continuum elastic theory based on the assumption that the film has an asymmetry between front and back, which can be attributed to the preparation conditions. We further present finite-element simulations of the twist, which show the dynamic shape change.

[1]Work supported by NSF DMR-0605889 and by ONR.

3:18PM W8.00005 Topography induced homeotropic alignment of nematic liquid crystals[1] , YOUNGWOO YI, NOEL CLARK, JOSEPH MACLENNAN, Department of Physics, The University of Colorado, Boulder, CO 80309, VAIBHAV KHIRE, CHRISTOPHER BOWMAN, Department of Chemical and Biological Engineering, The University of Colorado, Boulder, CO 80309 — We probe the orientation of a nematic liquid crystal on a planar aligning polymer film, where the film is topographically modified with sub micron scale checkerboard patterns. Alignment is studied in hybrid LC cells with the patterned polymer film on one plate and a self-assembled monolayer (homeotropic) on the other plate. A transition to homeotropic alignment on the pattern is observed as the pattern scale is reduced. An analysis shows that as the size of a square well becomes smaller the elastic energy of LCs decreases more slowly than the surface anchoring energy of the well, so that when the size of the well becomes small enough the elastic energy in planar configuration becomes comparable or larger than the polar anchoring energy of the surface.

[1]This work is supported by NSF MRSEC Grant DMR-0213918.

3:30PM W8.00006 Flexoelectric effect in a bent-core liquid crystal measured by Dynamic Light Scattering[1]

MADHABI MAJUMDAR, K. NEUPANE, JAMES. T. GLEESON, ANTAL JAKLI, SAMUEL SPRUNT, Kent State University — Flexoelectricity is a linear coupling between electric polarization and elastic flexure in liquid crystals [1]. Although typically quite weak in calamitic LCs, the flexoelectric effect has recently been shown, by direct (electromechanical) measurement of the flexure-induced polarization, to be enhanced by several orders of magnitude in certain bent-core nematic (BCN) liquid crystals [2]. We report here an application of dynamic light scattering to measure the flexoelectric coefficient ($e1 + e3$) of BCNs through coupling of polarization to elastic fluctuation modes of the optic axis. Our results agree in order of magnitude with the values obtained by the electromechanical method.

[1] R.B. Meyer, *Phys. Rev. Lett.* 22, 918 (1969).
[2] J. Harden, B. Mbanga, N. Eber, K. Fodor-Csorba, S. Sprunt, J. T. Gleeson, A. Jakli, *Phys. Rev. Lett.* 97, 157802 (2006).

[1]This work was financially supported by NSF Grant DMR- 0606160. We would like to thank J. Kim and W. Weissflog for synthesis of the bent-core material.

3:42PM W8.00007 Measurement of the Converse Flexoelectric Effect of a Bent-Core Nematic Liquid Crystal

JOHN HARDEN, Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, RICHELLE TEELING, SAMUEL SPRUNT, JAMES GLEESON, Department of Physics, Kent State University, ANTAL JAKLI, Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University — Flexoelectricity is a linear coupling between bend or splay distortions and electric polarization[1]. It is a unique property of orientationally ordered materials of which liquid crystals are the best known example. It has been shown that the bend flexoelectric coefficient in "banana" bent-core liquid crystals is three orders of magnitude higher than the effect found in calamitic liquid crystals[2]. Using a Mirau interferometer attached to the objective port of a microscope, we were able to measure the converse effect. This polarity dependent flexing of a thin cell yielded displacements of 100nm when 100V DC was applied to a 1cm x 2cm x 25μm cell filled with the bent-core nematic liquid crystal 4-chloro-1,3-phenylene bis 4-[4'-(9-decenyloxy) benzoyloxy] benzoate (ClPbis10BB). The substrates were 100μm thick Mylar with ITO as a conducting layer. These preliminary experiments show the promise of new types of soft actuators or beam steering devices. References: [1]Meyer R.B. (1969). Physical Review Letters **22**(18): 918-921. [2]Harden, J., B. Mbanga, et al. (2006). Physical Review Letters **97**(15). Acknowledgement: NSF DMR-0606160 and NSF REU-0649017

3:54PM W8.00008 Envelope Dynamics of an Experimental Electroconvection Pattern[1]

G. ACHARYA, Kent State University, G. DANGELMAYR, I. OPREA, Colorado State University, J.T. GLEESON, Kent State University — A video displaying electroconvection of the nematic I52 is analyzed. Spatial Fourier transforms of the frames reveal that the dynamics is driven by four groups of oblique (relative to the director) modes corresponding to counterpropagating pairs of traveling waves. This is consistent with a stability analysis of the electrohydrodynamic equations, which predict for I52 a Hopf bifurcation with four oblique critical wave numbers. Beyond the linear stability analysis, a weakly nonlinear analysis tells that the evolution of the pattern is governed by four slowly varying (in space and time) envelopes. These four envelopes are extracted from the pattern using Fourier analysis, and analyzed using several diagnostic tools such as statistical analysis, Karhunen Loeve decomposition, and the computation of correlation lengths and times as well as Lyapunov exponents. The results of this analysis indicate that the pattern shows extensive spatiotemporal chaos.

[1]Financially supported by NSF DMS-040721and DMS-0407418.

4:06PM W8.00009 Orientational order and topological defects on curved surfaces[1]

ROBIN SELINGER, JONATHAN SELINGER, Liquid Crystal Institute, Kent State Univ., ALEX TRAVESSET, Dept. of Physics and Astronomy, Iowa State Univ. and Ames Lab — Recent studies show a close relationship between geometry of surfaces and orientational order within the surfaces. Positive topological defects are attracted to regions of positive Gaussian curvature, and vice versa. To investigate this relationship, we develop a new computational approach to simulate orientational order on surfaces of arbitrary shape. We place xy spins on the surface in a disordered mesh constructed via random sequential absorption. We apply this approach to a sphere, a torus, and an "egg-crate" surface, $z = Asin(kx)sin(ky)$. For the sphere, we find a total topological charge of $+2$ as required by the Gauss-Bonnet theorem. For the torus, defects form in pairs, $+1$ defects on the outer edge (with positive Gaussian curvature) and -1 defects on the inner edge (with negative Gaussian curvature). For the egg-crate surface, with a coarse mesh, a $+1$ defect forms at each max/min and a -1 defect at every saddle point; while for a finer mesh, defects anneal away. We analyze these simulation results in terms of a continuum elastic model.

[1]Supported by NSF DMR-0605889 (R.S. and J.S.) , NSF DMR-0426597 (A.T.) , and the Institute for Complex Adaptive Matter.

4:18PM W8.00010 Local photo-reorientation of a liquid crystal using a laser focused on an azo dye-based monolayer[1]

YUE SHI, NOEL CLARK, Department of Physics and Liquid Crystal Material Research Center, University of Colorado at Boulder — The orientation adopted by molecules in an azobenzene-based self-assembled monolayer (azo-SAM) is perpendicular to the polarization of incident green light due to isomerization, aligning liquid crystal (LC) correspondingly. To study the local photo reorientation of the LC, the exciting laser is focused into a small spot on the azo-SAM, of a hybrid cell made with nematic LC sandwiched between the azo-SAM and a homeotropic surface. Under irradiation with changing polarization, a variety of interesting phenomena are observed, including winding of rings of reorientation and orientational slipping. Results vs. exciting light intensities and different rotating frequencies will be reported.

[1]Supported by NSF MRSEC Grant DMR-0213918

4:30PM W8.00011 Topology and Geometry of 1D Translational Order on Curved Surface[1]

XIANGJUN XING, Syracuse University — It is shown that one dimensional translational order on two dimensional curved substrate is naturally described by differential forms. A new type of global dislocation defects is identified and its relation with the topological properties of the embedding (compact) manifold is explored using algebraic topological methods. The associated topological charge classifies all ground states with no local defects. The energetics of smectic order on curved substrate is also discussed. Coupling between nematic director field and extrinsic curvature is shown to be important. As a simple application, the phase diagram of smectic order on a torus is analyzed. Two phases are identified: a small/thin phase where the nematic director is locked by curvature and a large/fat phase where the director varies continuously with system parameters.

[1]ACS PRF 44689-G7

4:42PM W8.00012 Coarsening of two-dimensional islands in freely suspended smectic A films[1]

, DUONG NGUYEN, CHEOL PARK, JOSEPH MACLENNAN, MATTHEW GLASER, NOEL CLARK, University of Colorado, Boulder — We have observed coalescence driven coarsening of islands (edge dilocation loops) in freely suspended Smectic A liquid crystal films. This is a good realization of a two-dimensional system, with films as thin as one molecular length (3-4 nm). The film is drawn by spreading material across a circular hole of about 4 mm in diameter, after which the film is suspended by the meniscus in contact with the edge of the hole. Islands are generated by blowing air parallel to the film surface, which produces a shearing force that breaks a thick region of the film into circular islands. Depending on the Smectic A material, we observe either strong or weak short-range repulsion between dislocation loops, leading to slow or fast coalescence, repectively. Over time, the average size of islands increases as the number of islands drops. The observed coasening dynamics is compared with theoretical predictions.

[1]Supported by NSF MRSEC Grant DMR-0213918 and NASA Grant NAG3-2457

4:54PM W8.00013 The Ground States of Nematic Order on a Sphere and Topological Defects

, HOMIN SHIN, MARK BOWICK, XIANGJUN XING, Syracuse University — We study the ground states of a spherical nematic order and the resulting configuration of topological defects. To emulate the ground state, we use hard rods confined on the surface of a sphere and very gradually compress the system upto the maximum packing density with Monte Carlo simulations. The nematic phases with four $+1/2$ disclination defects are clearly observed. Although the tetrahedral structure of four $+1/2$ defects is expected, we find all the defects most likely sitting on a great circle. The theoretical reasoning is provided with the calculation of defect energies in terms of the elastic anisotropy. Finally, we present that the allowance of some softness to the rods gives arise to qualitative changes in the director field surrounding the defect core.

5:06PM W8.00014 Thermal-Cycle Memory Functions and Ising Dynamics

, BRAD JOHNSON, DAVID PATRICK, Advanced Materials Science and Engineering Center, Western Washington University — The Ising model provides a rich system for the study of a variety of correlated systems. In this talk, we present the results of numerical studies of 2- and 3-dimensional Ising spin systems subjected to thermal cycling from an ordered state to states with a fixed order parameter (<1), but with differing overall morphologies, and back to a quenched state. We find that for systems with initial states generated by thermal disordering above T_c, the initial state of a given order parameter has larger 'islands' of like-spin (than the case for random disorder with the same overall order parameter) and consequent quenches of the state to $T<T_c$ result in a strong correlation to a particular final average order parameter. The function we find is given by $\langle S\rangle \approx \tanh(B \cdot S_{init})$, where S_{init} is the order parameter of the initial state, <S> is the average quenched order parameter, and B is a constant that depends upon the morphology of the initial state. The reason for the strong correlation stems from the energies associated with spins at the borders of large clusters. This 'memory effect' does not occur in 3D (due to the larger number of near-neighbors). Finally, we discuss the 'memory function' in the context of interfacial states of liquid crystals.

Friday, March 14, 2008 8:00AM - 10:48AM –

Session X8 DFD: Focus Session: Wormlike Micellar Fluids and Vesicles Morial Convention Center RO6

8:00AM X8.00001 Rheo-NMR of shear banded flow in wormlike micelles

, PAUL CALLAGHAN, Victoria University of Wellington — Rheo-NMR gives access to detailed information about the flow field generated by the device used to induce deformational flow. It also provides information about colloidal or molecular organisation and dynamics, under conditions of flow. In particular, NMR offers the possibility of measuring nuclear spin relaxation times and molecular self-diffusion coefficients, sensitive respectively to molecular brownian motions and their restrictions due to local structure. Furthermore, through the use of orientation-dependent terms in the spin interactions, such as the nuclear quadrupole or dipolar interactions, NMR permits the measurement of molecular order parameters. When combined with imaging methods, NMR in principle allows such measurements to be spatially localized, often with resolution down to a few 10s of microns In the study of shear banding phenomena in wormlike micelles, Rheo-NMR has proven of especial value, not only indicating the clear existence of shear bands, but also that they are associated with fluctuations, and sometimes, with molecular alignment. The subtlety of the correspondence (or lack of correspondence) between birefringence effects and shear banded flow has also been revealed. Recent measurements of shear-banded flow under Couette flow of the micellar system 10% w/v cetylpyridinium chloride and sodium salicylate (CPyCl/NaSal) molar ratio 2:1 in 0.5 M NaCl in ^1H_2O, indicate that shear banding fluctuations are consistent with the shear stress fluctuations observed in rheological measurements. Furthermore we find a coupling between flow fluctuations in the gradient and vorticity directions. Using ^{2}H NMR spectroscopy on a deuterated probe molecule (n-decane) in the wormlike micellar interior, direct measurement of the shear-induced nematic phase transition is reported. More recently we have used Rheo-NMR to investigate the flow and alignment properties of worm-like micelles formed by a 5% w/w solution of the BASF difunctional block copolymer non-ionic surfactant, Pluronic P105 in water along with 4.3% w/v 1-phenylethanol-d5. A variety of shear-banding and alignment behaviours are observed, along with both stable and fluctuating flows.

8:36AM X8.00002 Modeling the Inhomogeneous Response of Steady and Transient Flows of Entangled Micellar Solutions[1]

, GARETH MCKINLEY, MIT — Surfactant molecules can self-assemble in solution into long flexible structures known as wormlike micelles. These structures entangle, forming a viscoelastic network similar to those in entangled polymer melts and solutions. However, in contrast to 'inert' polymeric networks, wormlike micelles continuously break and reform leading to an additional relaxation mechanism and the name 'living polymers'. Observations in both classes of entangled fluids have shown that steady and transient shearing flows of these solutions exhibit spatial inhomogeneities such as 'shear-bands' at sufficiently large applied strains. In the present work, we investigate the dynamical response of a class of two-species elastic network models which can capture, in a self-consistent manner, the creation and destruction of elastically-active network segments, as well as diffusive coupling between the microstructural conformations and the local state of stress in regions with large spatial gradients of local deformation. These models incorporate a discrete version of the micellar breakage and reforming dynamics originally proposed by Cates and capture, at least qualitatively, non-affine tube deformation and chain disentanglement. The 'flow curves' of stress and apparent shear rate resulting from an assumption of homogeneous deformation is non-monotonic and linear stability analysis shows that the region of non-monotonic response is unstable. Calculation of the full inhomogeneous flow field results in localized shear bands that grow linearly in extent across the gap as the apparent shear rate increases. Time-dependent calculations in step strain, large amplitude oscillatory shear (LAOS) and in start up of steady shear flow show that the velocity profile in the gap and the total stress measured at the bounding surfaces are coupled and evolve in a complex non-monotonic manner as the shear bands develop and propagate.

[1]Joint work with L. Pamela Cook, Lin Zhou and Paula Vasquez, Research supported by NSF-DMS

9:12AM X8.00003 Rheology and Acoustics of Highly Concentrated Wormlike Micellar Fluids

, JOSEPH GLADDEN, JOEL MOBLEY, Dept. of Physics and Astronomy, University of Mississippi — Wormlike micellar fluids have long been studied as a model non-Newtonian fluid. The dynamic microstructure of the fluid gives rise to a rich diversity of hydrodynamic phenomenon. Generally, these fluids are studied in a low concentration regime (0-20 mM of surfactant). In this talk, we will discuss recent rheological and acoustic measurements of highly concentrated wormlike micellar fluids with concentrations of 50 - 400 mM cetyltrimethylammonium bromide (CTAB) and 30 - 240 mM (respectively) sodium salicylate (NaSAL) in the temperature range of 22 - 45 Celsius. In 200 mM CTAB fluids, the activation energy, derived from stress relaxation time measurements, exhibit a discontinuous shift from about 60 kT below 33 celsius to about 40 kT above. Speed of sound and acoustic attenuation measurements were obtained by a broadband Fourier spectroscopic method using ultrasonic waves between 2 and 8 MHz. Each of the concentrations measured exhibits an peak in the acoustic attenuation between 33 and 38 Celsius. The speed of sound increases monotonically over 22 - 40 Celsius, very similar to pure water in both magnitude and temperature dependence. Attenuation measurements as a function of acoustic power using high intensity focused ultrasound will also be discussed.

9:24AM X8.00004 The flow of wormlike micelles in microchannels: a micro-PIV study of shear-banding, interfacial instabilites and tracers migration , PHILIPPE NGHE, MMN, UMR CNRS-ESPCI Gulliver 7083, GUILLAUME DEGRE, LOF - UMR CNRS-Rhodia 5258, PATRICK TABELING, MMN, UMR CNRS-ESPCI Gulliver 7083, ARMAND AJDARI, PCT, UMR CNRS-ESPCI Gulliver 7083 — We characerize by Particle Image Velocimetry the Poiseuille flow a semi-dilute solution of wormlike micelles (a CTAB and sodium nitrate aqueous solution) in pressure resistant microchannels. Thanks to the high aspect ratio of our channels, we can measure the local rheology of the solution, independantly from the slippage at the wall, according to a method already validated on non-newtonian polymer solutions. As the pressure driving the flow is increased, the velocity profiles reveal first a newtonian phase, then apparition of a dramatically lower viscosity second phase at the walls, which is the so called shear banding regime. First we deduce the local rheology of the solution from these velocity profiles, in agreement with the macroscopic rheology obtained in Couette rheometers. Then we study the development of an instability at the interface between the two phases, with a wavevector in the vorticity direction and a wavelength corresponding to smallest dimension of the channel. Finally we discuss the hypothesis of passive tracers : depending on their size, we observe a tracer depletion in the high-shear phase, which may be to high normal forces.

9:36AM X8.00005 Reversible and irreversible flow-induced phase transition in micellar solutions[1] , RADHAKRISHNA SURESHKUMAR[2], MUKUND VASUDEVAN, ERIC BUSE, Washington University in Saint Louis, HARE KRISHNA, RAMKI KALYANARAMAN, Washington University in Saint Louis, BAMIN KHOMAMI, University of Tennessee, Knoxville, AMY SHEN, Washington University in Saint Louis — It is well known that wormlike micelles form shear-induced structures (SIS). SIS formation is typically accompanied by the appearance of a gel-like phase. While both configurational dynamics of the micelles in flow and electrostatics are recognized as the key factors that influence such phase transitions, there are no universally applicable criteria for the onset strain rate as function of salt concentration. In this work, first, we examine the effect of salt concentration on the critical strain rate for CTAB/NaSal solutions and show that a "self-similar" phase transition regime exists. Second, we show that under strong (elongational) flow conditions, the phase transitions are irreversible, leading to the formation of gels that are stable even after the flow is stopped. Results obtained from atomic force microscopy studies of the structure of such gels will be presented.

[1]NSF
[2]Corresponding Author

9:48AM X8.00006 Investigating the structures and phase behavior of anionic perfluorinated surfactant using SANS , GARFIELD WARREN, DOBRIN BOSSEV, Indiana University — We have examined the structures formed by mixtures of tetraethylammonium perfluorooctylsulfonate (TEAFOS) and lithium perfluorooctylsulfonate (LiFOS) in water using small angle neutron scattering (SANS). SANS is an ideal method to characterize the morphology of such soft materials because the wavelength of the cold neutrons is comparable to the characteristic length scale of the surfactant structures and the possibility to apply the contrast variation technique. Results were obtained for mixtures at a constant surfactant concentration of 100 mM and different TEA/Li ratios at a temperature of 30°C. SANS curves were obtained either from the fluorinated micellar core or from the hydrogenated counterion atmosphere surrounding the micelles applying contrast matching. A transitional change in shape from spherical to prolate micelles was observed for TEA fractions greater than 30 mM. For TEA fractions greater than 55mM, threadlike micelle structures are present. From the SANS data we are able to correlate the counterion binding of the two different species to the shape and size of the micellar structure and confirm the role that the counterion environment plays in macroscopic rheological properties.

10:00AM X8.00007 Fabrication of phospholipid vesicles from double emulsions in microfluidics , INSUN YOON, Mount Holyoke College, ANDERSON H. SHUM, DAEYEON LEE, DAVID A. WEITZ, School of Engineering and Applied Sciences, Harvard University — Phospholipids self-assemble into lipid vesicles also known as liposomes. The formation of liposomes via conventional techniques such as electroformation has been studied extensively. However, the liposomes formed through electroformation are polydisperse and have low encapsulation efficiency. We present a new method to fabricate monodisperse phospholipid vesicles with high encapsulation efficiency from water-in-oil-in-water double emulsions. We generate phospholipid stabilized monodisperse double emulsions using a glass microcapillary device. This process allows efficient encapsulation within the inner aqueous drop. The middle oil phase is a volatile organic solvent in which phospholipids are dissolved. As the organic solvent evaporates, phospholipids self-organize into vesicles. This technique is versatile in the choice of phospholipids and we have generated vesicles from different types of phospholipids.

10:12AM X8.00008 Concentration dependence of dynamics of a droplet microemulsion , MICHIHIRO NAGAO[1], Indiana University, HIDEKI SETO, Kyoto University, Japan — We will present a concentration dependence of dynamics of a spherical droplet microemulsion, consisting of aerosol-OT (AOT), as a surfactant, water, and decane. This mixture forms spherical microemulsion in a wide range of concentration. With keeping water to surfactant ratio constant, concentration of water plus surfactant was changed. The static structure of this system has been determined by small-angle neutron scattering (SANS) using the relative form factor method in the droplet concentration range from 5 to 75 % [1]. Dynamics of droplet microemulsions have been determined using neutron spin echo technique, which is suitable to measure dynamics of systems in nanometer and nanosecond scales. We measured dynamics of the system at 5, 30, and 60 % of droplet concentration. Using analogous data reduction procedure to SANS, contribution of shape fluctuations is decoupled from structure fluctuations. Concentration dependence of shape fluctuations and structure fluctuations will be discussed. [1] M. Nagao et al., Phys. Rev. E 75, 061401 (2007).

[1]Also at National Institute of Standards and Technology

10:24AM X8.00009 Dielectrophoresis of Functional Phospholipid Vesicles , VICTORIA FROUDE, YINGXI ELAINE ZHU, University of Notre Dame — Recently, there has been an emerging interest in using AC-dielectrophoresis (DEP) to transport and assemble phospholipid vesicles (liposomes) and nanoparticles to form functional bio-assemblies where the underlying charge polarization mechanism of colloids in AC fields strongly depends on nano-scaled surface charge. In this work, we study liposomes segregation and aggregation in the presence of nanocolloids and salts in which the biological functionality of liposomes is augmented by the physical functionality of inorganic coating and particles. Liposomes, synthesized by sonication with 1,2-Dioleoyl-sn-Glycero-3-Phosphate (DOPA), are manipulated at varied AC-field frequencies across fabricated micro-electrodes in a quadrapole configuration on glass. We observe the co-assembly of liposome and opposite-charged nanocolloids by confocal microscopy and SEM, where the smaller nanocolloids are captured in between liposome junctions to form stabilized composite vesicles at several distinct frequencies. We observe a strong dependence of the liposome DEP mobility on the number of nanoparticles present in suspension and propose a new mechanism based on charge segregation and charged nanocolloid entrainment in the double layer.

10:36AM X8.00010 High-throughput Microsphere Encapsulation in Emulsion Droplets by Electrospray , WUEN-SHIU CHEN, KENG-HUI LIN, Institute of Physics, Academia Sinica, Tapei, Taiwan — Colloidal clusters generated through emulsion encapsulation and evaporation open up the possibilities for assembly of complex crystal structures. Encapsulation in monodisperse emulsion droplets facilitates higher yield of identical clusters as building blocks. We utilize electrospray in an oil-in-water co-flow fluidic device to generate uniform emulsion droplets in micron size and at the rate of ten thousand droplets per second. We investigate the effect of applied voltage, flow rate and the conductivity of liquid on the droplet formation. We further show that incorporation of microspheres into the inner oil fluid enables the encapsulation and formation of clusters.

Friday, March 14, 2008 11:15AM - 1:39PM –

Session Y8 DFD: Hydrodynamics of Surfaces and Films Morial Convention Center RO6

11:15AM Y8.00001 Capillary ratchet: Hydrodynamics of capillary feeding in shorebirds[1]

, MANU PRAKASH, MIT, DAVID QUERE, ESPCI, Paris, JOHN BUSH, MIT — Bill morphologies are highly specialized to particular foraging strategies in birds, as is apparent from the large diversity of beak shapes observed in nature. Here we present an experimental and analytical study of capillary feeding in shorebirds. We highlight the critical role of contact angle hysteresis in capillary feeding. Our study provides a simple physical rationalization for the observation of multiple mandibular spreading cycles in feeding, necessary to overcome contact line resistance. We also find a unique geometrical optima in beak opening and closing angles for the most efficient drop transport. This capillary ratchet mechanism may also find applications in micro scale fluid transport, such as valveless pumping of fluid drops.

[1]Center for Bits and Atoms, MIT.

11:27AM Y8.00002 Rheology and Microrheology of Actin-Lipid Composites at the Air-Water Interface[1]

, ROBERT WALDER, University of California, Irvine, ALEX LEVINE, University of California, Los Angeles, CHRISTOPH SCHMIDT, Third Physical Institute: Biophysics Georg-August-Universität, Göettingen, Germany, MICHAEL DENNIN, University of California, Irvine — We report on the mechanical properties of a composite material that is a combination of a Langmuir monolayer chemically linked to an actin filament network. This composite system is a 2 dimensional analogue of a cellular membrane and is also expected to have interesting nonlinear mechanical properties. To measure these mechanical properties, we employ traditional rheology and have developed unique microrheological capabilities based on an optical tweezer setup combined with a Couette surface rheometer. This combination of techniques will allow the study of both bulk and local mechanical responses of the composite material to external forces. Studying such materials allows us to simultaneously study a biomimetic material that should provide useful insights into the mechanical properties of biological cells, while also providing a 2 dimensional soft matter system to study the properties of semi-flexible polymer networks.

[1]Supported by NSF-DMR-0354113. R Walder acknowledges support from a travel fellowship from Institute for Complex Adaptive Matter

11:39AM Y8.00003 ABSTRACT WITHDRAWN –

11:51AM Y8.00004 Elasticity and capillarity: wet hairs and origami

, JOSÉ BICO, LINGGUO DU, BENOIT ROMAN, PMMH-ESPCI, JEROME GUILET, ENS, Paris — Capillary forces are responsible for a large range of everyday observations : the shape of rain droplets, the imbibition of a sponge, the clumping of wet hair into bundles. Although they are often negligible on macroscopic structures, surface capillary forces may overcome volume forces at small scales and deform compliant micro-structures. Capillary-induced sticking can prevent the actuation of mobile elements in MEMS, or even cause their collapse. Capillary forces also have important consequences in biology such as the buckling of the airway lumen induced by surface tension, which can eventually cause the lethal closure of lung airways. We will review a few experimental situations where capillary forces are able to deform two types of objects: rods, and thin sheets. For instance, the nanotubes of a "carbon nanotube carpet" self-assemble into conical "teepee" structures after the evaporation of a solvent and can produce intriguing cellular patterns. Similarly macroscopic wet hairs tend to assemble into bundles through a cascade of successive pairings. The comparison of the physical ingredients involved in these phenomena, attracting capillary forces acting against bending elasticity, leads to a characteristic length: a slander structure longer than this "elasto-capillary" length is considerably bent by capillary forces. The case of thin sheets is trickier because of geometrical constrains, which generally leads to singularities.

12:03PM Y8.00005 Flow fields in soap films: effects of surface viscosity and film thickness

, VIKRAM PRASAD, ERIC R. WEEKS, Emory University — A soap film is a thin fluid layer (10 nm to 10 microns thick) separated from bulk air phases above and below it by two surfactant monolayers. We measure the flow field in these films by two-particle microrheology, which looks at the correlated Brownian motion of pairs of embedded tracer particles separated by a distance R. In thin soap films with the thickness comparable to the particle size, and with mobile surfactant interfacial layers, this flow field is long ranged. On the other hand, the flow field in a 3D fluid is known to decay as 1/R. We vary the thickness of the soap film, the mobility (surface viscosity) of the interface and the size of the polystyrene probe particles to quantify the transition of the hydrodynamics of the film from quasi-2D to 3D-like behavior.

12:15PM Y8.00006 Effective Viscosity of a Dilute Suspension of Membrane-bound Inclusions

, MARK L. HENLE, ALEX J. LEVINE, Department of Chemistry and Biochemistry, University of California, Los Angeles — In 1906, Einstein famously calculated the effective viscosity of a dilute solution of spheres suspended in a viscous solvent [*Annalen der Physik* **19**, 289 (1906)]. In this talk, we consider the two-dimensional analogue of this problem: that is, we calculate the effective viscosity of a dilute suspension of disks embedded in a two-dimensional fluid membrane. The rheological properties of particle-decorated membranes and fluid-fluid interfaces are important in a variety of soft matter systems. For example, the cell membrane contains a suspension of membrane-bound inclusions (e.g. transmembrane proteins, lipid rafts), which modifies the transport kinetics of the membrane. Also, the interfacial viscosity of liquid-liquid interfaces in colloid-stabilized emulsions plays a key role in preventing droplet coalescence. We include the dissipation caused by flows both within the membrane and in the surrounding bulk fluids. When the flows within the membrane dominate the dissipation, the particle suspension effectively shifts the membrane viscosity. Conversely, when flows induced in the bulk fluids dominate the dissipation, the suspension in the membrane shifts the bulk viscosity. In both limits, we obtain simple analytic expressions for the appropriate effective viscosity.

12:27PM Y8.00007 Contact line motions of drying solutions

, FRANCOIS LEQUEUX, CECILE MONTEUX, ASTRID TAY, PPMD/ESPCI, EMMANUELLE RIO, LPS/ORSAY, LAURENT LIMAT, GUILLAUME BERTELOOT, ADRIEN DAERR, MSC/PARIS, PPMD/ESPCI/PARIS TEAM, LPS/ORSAY/FRANCE TEAM, MSC/PARIS/FRANCE TEAM — If most the studies on wetting deal with pure liquids in the absence of evaporation, in practical situations, the liquid is often a solution with an evaporating solvent. This is encountered both in coating and in surface cleaning. In that case, the contact line of a solution is the location of many divergent phenomena. The hydrodynamics dissipation diverges at the contact line: 1) the drying rate diverges at the contact line 2) the concentration diverges at the contact line. The coupling of these phenomena leads to complex effect for the contact line motion. We have observed that an advancing contact line of a colloidal suspension exhibit a stick-slip motion. Moreover, for similar reasons in the case, an advancing contact line of a polymer solution, the contact angle exhibit a minimum as a function of velocity – at which the polymer accumulates on a length of typically 5 nm in the vicinity of the contact line. All these phenomena can explained quantitatively using simple scaling arguments that we will present.

12:39PM Y8.00008 Obtaining Reproducible Slip Measurements on Smooth Hydrophobic Surfaces , SEAN P. MCBRIDE, B.M. LAW, Kansas State University — Over the past decade, the world market for microfluidic technologies and applications of such devices has soared. The slip length parameter at the liquid-surface interface of these devices describes how easily a fluid flows over the surface. As microfluidic devices decrease in size, slip becomes very important. Despite the undeniable success of these devices in recent years, the literature illustrates that numerous discrepancies exist for the slip magnitude measured using different experimental methods. As the need for smaller microfluidic devices approaches a consistent experimental method is needed to obtain reproducible slip results. The method employed to study slip, in this research, uses an Atomic Force Microscope (AFM) to obtain the hydrodynamic force exerted on a colloidal cantilever which is immersed in a homologous series of test liquids and driven toward a smooth hydrophobic surface. The surfaces are prepared using silicon wafers with 0.4nm RMS over a 5x5um area and coated with hexadecyltricholorsilane (HTS) via cold liquid deposition. This method provides reliable and reproducible slip measurements that are consistent with a constant slip length over a wide shear rate range. This research was supported by NSF grant DMR-0603144.

12:51PM Y8.00009 Fabrication of non-aging superhydrophobic surfaces by packing flower-like hematite particles , ANMIN CAO, LIANGLIANG CAO, DI GAO, University of Pittsburgh — We demonstrate the fabrication of non-aging superhydrophobic surfaces by packing flower-like micrometer-sized hematite particles. Although hematite is intrinsically hydrophilic, the nanometer-sized protrusions on the particles form textures with overhanging structures that prevent water from entering into the textures and induce a macroscopic superhydrophobic phenomenon. These superhydrophobic surfaces do not age even in extremely oxidative environments—they retain the superhydrophobicity after being stored in ambient laboratory air for 4 months, heated to 800 degree C in air for 10 hours, and exposed to ultraviolet ozone for 10 hours.

1:03PM Y8.00010 Liquid slip probed by second harmonic generation[1] , DAN LIS, Laboratoire Lasers & Spectroscopies, University of Namur, STEVE GRANICK, BAE SUNG CHUL, Departments of Materials Science and Engineering, Chemistry, and Physics, University of Illinois, SCIENTIFIC EXCHANGE COLLABORATION — Second harmonic generation has been used to probe how a solid surface responds to flow past it. The surface is quartz, the measurements are made in total internal reflection configuration, and comparison of responses to light with s and p incident polarisation allows us to determine the orientation of dye molecules physisorbed before the onset of the shear flow. By monitoring the orientation of the dye at different fluid viscosity and different shear rate, we deduce the surprising relation between shear rate and surface stress.

[1]Dan Lis acknowledges the Belgian Fund for Agricultural and Industrial Research (FRIA) for financial support.

1:15PM Y8.00011 Determination of Inter-Phase Line Tension in Langmuir Films[1] , ELIZABETH K. MANN, LU ZOU, Kent State University, JACOB R. WINTERSMITH, ANDREW J. BERNOFF, Harvey Mudd College, JAMES C. ALEXANDER, J. ADIN MANN, JR., Case Western Reserve University, PREM BASNET, EDGAR E. KOOIJMAN, Kent State University — The hydrodynamic response of a thin fluid film, whether a Langmuir monolayer at the air/water interface or a cell membrane, is difficult to model, since it involves the coupling of both bulk and surfaces phases. However, such hydrodynamic response is not only intrinsically critical for transport within the layer, it also provides the major available means to evaluate an important parameter for phase-separated layers, the line tension. We have developed a line-integral formulation of the hydrodynamic response of phase-separated layers with short-ranged forces, and tested it by comparisons between numerical simulations based on this model and experiment. These experiments both validate the model and demonstrate that the line tension can be determined with unprecedented accuracy and precision. Two systems have been studied to date: a simple smectic liquid crystal multilayer and coexistence between phases in binary lipid/cholesterol mixed layers. For the latter case, long-range dipole-dipole interactions are introduced into the model.

[1]This work is partially supported by the NSF grant CBET-0730475.

1:27PM Y8.00012 ABSTRACT WITHDRAWN –