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Monday, March 21, 2011 8:00AM - 11:00AM – Session A9 DFD: Micro-fluidics D220

8:00AM A9.00001 Hydrodynamic resistance of confined cells in rectangular microchannels

ZEINA S. KHAN, SIVA A. VANAPALLI, Texas Tech University, Department of Chemical Engineering — Several microfluidic approaches have been developed to screen suspended cells mechanically in microchannels by exploiting characteristics that are linked to their individual mechanical properties. Typically changes in cell shape due to shear-induced deformation and transit times are reported; while these measurements are qualitative compared to more precise techniques such as atomic force microscopy and micropipette aspiration their advantage lies in throughput, with the ability to screen hundreds to thousands of cells in a minute. We study the potential of a microfluidic cell squeezer to characterize the hydrodynamic resistance of LNCaP prostate cancer cells by measuring dynamical pressure-drop variations along a micrometer-sized channel. The hydrodynamic resistance of the cell introduces an excess pressure drop in the narrow channel which depends on the mechanical stiffness of the cell. We additionally visualize the cell size and assess the influence of cell size on the hydrodynamic resistance of each cell, demonstrating the capability of the microfluidic cell squeezer to yield the hydrodynamic resistance as a mechanical fingerprint of cells.

8:12AM A9.00002 Bio-inspired artificial iridophores based on capillary origami

SUPONE MANAKASETTARN, J. ASHLEY TAYLOR, TOM KRUPENKIN, University of Wisconsin - Madison — Many marine organisms have evolved complex optical mechanisms of dynamic skin color control that allow them to drastically change their visual appearance. In particular, cephalopods have developed especially effective dynamic color control mechanism based on the mechanical actuation of the micro-scale optical structures, which produce either variable degrees of area coverage by a given color (chromatophores) or variations in spatial orientation of the reflective and diffractive surfaces (iridophores). In this work we describe bio-inspired artificial iridophores based on electrowetting-controlled capillary origami. We describe the developed microfabrication approach, characterize mechanical and optical properties of the obtained microstructures and discuss their electrowetting-based actuation. The obtained experimental results are in good agreement with a simple theoretical model based on electrocapillarity and elasticity theory. The results of the work can enable a broad range of novel optical devices.

8:24AM A9.00003 Micropipette as Coulter counter for submicron particles¹

YAUHUNI RUDZEVICH, TONY ORDONEZ, GRANT EVANS, LEE CHOW, University of Central Florida — Coulter counter based on micropipette has been around for several decades. Typical commercial Coulter counter has a pore size of 20 μm , and is designed to detect micron-size blood cells. In recent years, there are a lot of interests in using nanometer pore size Coulter counter to detect single molecule and to sequence DNA. Here we describe a simple nanoparticle counter based on pulled micropipettes with a diameter of 50 – 500 nm. Borosilicate micropipettes with an initial outer diameter of 1.00 mm and inner diameter of 0.5 mm are used. After pulling, the micropipettes are fire polished and ultrasound cleaned. Chlorinated Ag/AgCl electrodes and 0.1 M of KCl solution are used. The ionic currents are measured using an Axopatch 200B amplifier in the voltage-clamp mode. Several types and sizes of nanoparticles are measured, including plain silica and polystyrene nanospheres. The results will be discussed in terms of pH values of the solution and concentrations of the nanoparticles.

¹Financial support from National Science Foundation (NSF-0901361) is acknowledged.

8:36AM A9.00004 ABSTRACT WITHDRAWN –

8:48AM A9.00005 On demand fusion and triggering of confined chemical reactions in femtoliter volume aqueous droplets controlled by interfacial tension

PAT COLLIER, SEUNG-YONG JUNG, SCOTT RETTERER, ORNL — Droplet-based microfluidic platforms offer many opportunities to confine chemical and biochemical reactants in discrete ultrasmall reaction volumes, and investigate the effects of increased confinement on reaction dynamics. Current state-of-the-art microfluidic sampling strategies for creating ultrasmall reaction volumes are predominately steady-state approaches, which result in difficulty in trapping reacting species with a well-defined time-zero for initiation of biochemical reactions in the confined space. This talk describes stepwise, on-demand generation and fusion of femtoliter aqueous droplets based on interfacial tension. Sub-millisecond reaction times from droplet fusion were demonstrated, as well as a reversible chemical toggle switch based on alternating fusion of droplets containing acidic or basic solution, monitored with the pH-dependent emission of fluorescein.

9:00AM A9.00006 Acoustic actuation and sorting of droplets and cells at ultrahigh rates in microfluidics

THOMAS FRANKE, Harvard University/University of Augsburg, LOTHAR SCHMID, SUSANNE BRAUNMUELLER, ACHIM WIXFORTH, University of Augsburg, DAVID A. WEITZ, Harvard University, FRANKE TEAM, FRANKE/WEITZ TEAM — We direct the motion of droplets in microfluidic channels using a surface acoustic wave device. This method allows individual drops to be directed along separate microchannel paths at high volume flow rates, which is useful for droplet sorting. The same principle can be applied for biological cell sorting which operates in continuous flow at high sorting rates. The device is based on a surface acoustic wave cell-sorting scheme and combines many advantages of fluorescence activated cell sorting (FACS) and fluorescence activated droplet sorting (FADS) in microfluidic channels. It is fully integrated on a PDMS device, and allows fast electronic control of cell diversion. We direct cells (HaCaT, MV3 melanoma, fibroblasts) by acoustic streaming excited by a surface acoustic wave. The device underlying principle works without additional enhancement of the sorting by prior labeling of the cells with responsive markers such as magnetic or polarizable beads. We have combined the acoustic device successfully with a laser based fluorescence detection system and demonstrate sorting of fluorescent labeled drops at rates of several kHz without any false sorting.

9:12AM A9.00007 Microfluidic mixing using an array of superparamagnetic beads

WENBIN MAO, ZHENGCHUN PENG, PETER J. HESKETH, ALEXANDER ALEXEEV, Georgia Institute of Technology — We present a combined numerical and experimental study on the dynamics of superparamagnetic beads in a microfluidic channel, wall of which is decorated with an array of stationary magnetic disks. When exposed to a rotating magnetic field, the beads circulate around the magnetic disks. We conduct experiments with micrometer-sized superparamagnetic beads and use a numerical method that is based on the lattice Boltzmann model to examine the dynamics of this microfluidic system. We isolate the conditions in which beads exhibit stable periodical motion around magnetic disks and probe the effect of microchannel flow on the bead dynamics. We demonstrate that the fluid circulations created by rotating beads can be exploited for microfluidic mixing, thereby offering a new approach for designing highly-efficient active microfluidic mixers.

9:24AM A9.00008 Separating Magnetically Labeled and Unlabeled Biological Cells within Microfluidic Channels

TOM BYVANK, GREG VIEIRA, The Ohio State University Department of Physics, BRANDON MILLER, BO YU, JEFFREY CHALMERS, L. JAMES LEE, The Ohio State University William G. Lowrie Department of Chemical and Biomolecular Engineering, R. SOORYAKUMAR, The Ohio State University Department of Physics — The transport of microscopic objects that rely on magnetic forces have numerous advantages including flexibility of controlling many design parameters and the long range magnetic interactions generally do not adversely affect biological or chemical interactions. We present results on the use of magnetic micro-arrays imprinted within polydimethylsiloxane (PDMS) microfluidic channels that benefit from these features and the ability to rapidly reprogram the magnetic energy landscape for cell manipulation and sorting applications. A central enabling feature is the very large, tunable, magnetic field gradients ($> 10^4$ T/m) that can be designed within the microfluidic architecture. Through use of antibody-conjugated magnetic microspheres to label biological cells, results on the transport and sorting of heterogeneous cell populations are presented. The effects of micro-array and fluid channel design parameters, competition between magnetic forces and hydrodynamic drag forces, and cell-labeling efficiency on cell separation are discussed.

9:36AM A9.00009 Coating microchannels to improve Field-Flow Fractionation, TYLER N. SHENDRUK, GARY W. SLATER, University of Ottawa — We propose a selective-steric-mode Field-Flow Fractionation (ssFFF) technique for size separation of particles. Grafting a dense polymer brush onto the accumulation wall of a microchannel adds two novel effects to FFF: the particles must pay an entropic cost to enter the brush and the brush has a hydrodynamic thickness that shifts the no-slip condition. For small particles, the brush acts as a low-velocity region, leading to chromatographic-like retention. We present an analytical retention theory for small but finite-sized particles in a microchannel with a dense Alexander brush coating that possesses a well-defined hydrodynamic thickness. This theory is compared to a numerical solution for the retention ratio given by a flow approximated by the Brinkman equation and particle-brush interaction that is both osmotic and compressional. Large performance improvements are predicted in several regimes. Multi-Particle Collision simulations of the system assess the impact of factors neglected by the theory such as the dynamics of particle impingement on the brush subject to a flow.

9:48AM A9.00010 Digital Flow Control of Electroosmotic Pump: Onsager Coefficients and Interfacial Parameters Determination, ZULI XU, Department of Physics, the Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong (PR China), JIANYING MIAO, Nano and Advanced Materials Institute Limited, Hong Kong (PR China), NING WANG, PING SHENG, Department of Physics, the Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong (PR China) — Electroosmosis (EO) and streaming potential (SP) are two complementary electrokinetic processes related by the Onsager relation. In particular, electroosmotic pump (EOP) is potentially useful for a variety of engineering and bio-related applications. By fabricating samples consisting of dry-etched cylindrical pores (50 μm in length and 3.5 μm in diameter) on silicon wafers, we demonstrate that the use of digital control via voltage pulses can resolve the flow regulation and stability issues associated with the EOP, so that the intrinsic characteristics of the porous sample medium may be revealed. Through the consistency of the measured electroosmosis and the streaming potential coefficients as required by the Onsager relation, we deduce the zeta potential and the surface conductivity, both physical parameters pertaining to the liquid-solid interface.

10:00AM A9.00011 AC electrophoretic effect in inhomogeneous electrical field: potentials for single molecule trapping¹, WEIHUA GUAN, Department of Electrical Engineering, Yale University, JAE HYUN PARK, PREDRAG KRSTIC, Physics Division, Oak Ridge National Laboratory, MARK REED, Department of Electrical Engineering, Yale University — In micro-fabricated fluidic devices, we have experimentally observed trapping of objects in the supposed unallowed positive dielectrophoresis (pDEP) region. This 'anomalous' trapping behavior motivates us to investigate the missing contributions in the trapping dynamics. We present here a study on overlooked aspects of alternating current (AC) electrokinetics-AC electrophoretic (ACEP) phenomena. The dynamics of a particle with both polarizability and net charges in an *inhomogeneous* AC electric trapping field are investigated. It is found that either electrophoretic (EP) or dielectrophoretic (DEP) effects can dominate the trapping dynamics, depending on experimental conditions. A dimensionless parameter is developed to predict the relative strength of EP and DEP effect. Contrary to conventional thought, an ACEP trap is feasible for charged particles in 'salt-free' or low salt concentration solutions. In contrast to DEP traps, an ACEP trap favors the down scaling of particle size. We anticipate that this feature will allow the confinement of single nanometer-sized objects or macromolecules.

¹Supported by NIH under grant No. 1R21HG004764-01

10:12AM A9.00012 Making robust electrowetting processes: dielectric breakdown and satellite droplets, GREG RANDALL, BRENT BLUE, General Atomics — For over ten years, charge-related wetting phenomena such as electrowetting or dielectrophoresis have been used to manipulate individual liquid droplets on grids of patterned electrodes. Many proof-of-principle droplet actuations have been shown, however some physics-based problems are complicating this technology's move to industry. These problems include: breakdown of a device's dielectric coating at field strengths lower than anticipated and generation of satellite droplets from the primary droplet's surface. We use atomic layer deposition (ALD) to fabricate high-quality dielectric layers required for robust droplet electrowetting and generate operating plots for several dielectric materials. Using scanning electron microscopy and X-ray spectroscopy, we study damage and ionic penetration into the device's dielectric layer. Using video and current measurements, we examine the physics of satellite droplet generation. We apply these findings to engineer a microfluidic process to mass produce inertial fusion energy targets.

10:24AM A9.00013 Introducing the Hybrid Free Surface Microfluidics for Gas Sensing, MEYSAM BARM, CARL MEINHART, Department of Mechanical Engineering, University of California Santa Barbara — Free-Surface Microfluidics (FSMF) have recently received much attention for their applications especially their ability for airborne chemical detection [Piorek, PNAS 2007]. Due to their sensitivity to the ambient condition and possibility of contamination, hybrid configuration is introduced to perform the measurement more accurately. The hybrid free surface microfluidics are combination of free surface and closed surface microfluidics. The gas is absorbed by the working fluid through a small opening on the microchannel and transported to the closed surface reaction chamber to carry out the measurements. The working fluid is transported by surface tension and regulated by temperature-controlled evaporator at the outlet. The microchannels are fabricated on Silicon substrates with built-in Ti/Pt electrodes to measure the conductivity of the working fluid before and after the gas absorption to find the concentration of the absorbed gas. It proves that the hybrid free surface microfluidics are appropriate for gas sensing and the minimum exposing time and required opening size are calculated. Numerical simulations are carried out by COMSOL multiphysics. Navier-Stokes equations along with the mass transport with reaction are solved simultaneously to find the correlation between vapor pressure of the surrounding gas and concentration of the absorbed gas.

10:36AM A9.00014 Motion-Reversal Transitions in Self-Assembled Colloidal Walkers, STEPHANIE MORAN, CHARLES SING, ALFREDO ALEXANDER-KATZ, MIT — Nature has created a variety of designs in order to move fluids and transport objects within living organisms. At microscopic scales (in the region of micrometers) two motifs are common: flagella and cilia. Within the cell, however, molecular motors with nanometer dimensions transport small sized vesicles. Here, we describe a novel approach that combines properties from two systems: cilia and molecular motors, to create self-assembled colloidal walkers. These walkers are assembled by superparamagnetic beads in the presence of a rotating homogeneous magnetic field, and are able to move in a given direction due to the presence of surfaces which provide an effective friction. The motion is somewhat reminiscent of a person doing cartwheels on ice, where the friction is not high enough to avoid slip, but overall one can attain directed motion in one direction. Interestingly, the motion of the center of mass of these walkers is a non-monotonic function along one cycle of revolution. By exploiting this non-monotonicity, we show that motion reversal is possible in these systems if one carefully controls the friction properties of the surface as well as the confining "gravitational" field that maintains the beads near the surface. Our results are important in understanding the motion of micron scale organisms and may be useful in the development of virtual microfluidic platforms.

10:48AM A9.00015 Optimizing Nanopore Surface Properties for High-Efficiency Water Desalination, DAVID COHEN-TANUGI, JEFFREY GROSSMAN, Massachusetts Institute of Technology — As water resources worldwide become rapidly scarcer, it is becoming increasingly important to devise new techniques to obtain clean water from seawater. At present, water purification technologies are limited by costly energy requirements relative to the theoretical thermodynamic limit and by insufficient understanding of the physical processes underlying ion filtration and fluid transport at the molecular scale. New advances in computational materials science offer a promising way to deepen our understanding of these physical phenomena. In this presentation, we describe a new approach for high-efficiency water desalination based on surface-engineered porous materials. This approach is especially relevant for promising technologies such as nanofiltration and membrane distillation, which offers promising advantages over traditional desalination technologies using mesoporous membranes that are only permeable to pure water vapor. More accurate molecular modeling of mesoporous and nanoporous materials represents a key step towards efficient large-scale treatment of seawater. Results regarding the effect of pore properties (surface texture, morphology, density, tortuosity) on desired performance characteristics such as ion selectivity, maximal water flux and energy requirements will be presented.

Monday, March 21, 2011 8:00AM - 11:00AM –

Session A13 DFD DPOLY: Focus Session: Polymer Colloids: Structure, Function, and Dynamics | D225/226

8:00AM A13.00001 Osmotic pressure of microgel suspensions, JUAN JOSE LIETOR-SANTOS, BENJAMIN SIERRA-MARTIN, JUSTIN FREDERICK, YESENIA LAPORTE, GEORGE MARKOU, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Microgels are crosslinked-polymeric networks in the colloidal domain, whose size can change in response to external stimuli. They are soft particles by construction and can exhibit a very different behavior compared to hard sphere suspensions. In some cases, this different behavior has been understood by alluding to particle de-swelling at low volume fractions. For this to happen, the suspension osmotic pressure at such volume fraction should be comparable to the particle bulk modulus. In this work, we independently measure the bulk modulus of microgel particles and the suspension osmotic pressure and find that both magnitudes become comparable at a volume fraction corresponding to a liquid-to-solid transition, which we assess using rheology. Interestingly, in the solid region, the shear and compressional moduli of the suspension exhibit the same behavior with volume fraction, in analogy to emulsions. However, by contrast to emulsions, they are almost two orders of magnitude apart. This reflects the contributions from the internal modes of the microgel particles, which are absent for the case of an emulsion drop.

8:12AM A13.00002 Particle Charging and Interaction in Nonpolar Colloidal Dispersions Mediated by Nonionic Surfactants, SVEN BEHRENS, Georgia Tech — The electrostatic stabilization of colloidal dispersions is usually considered the domain of polar media only, but some surfactants are known to raise the conductivity of liquids with low electric permittivity and to mediate charge-stabilization of nonpolar dispersions. Here we report an example of the counterintuitive electrostatic effects of nonionic surfactants on colloidal particles in nonpolar solvents. PMMA particles in hexane solutions of sorbitan oleate (Span) surfactants exhibit a field-dependent electrophoretic mobility. In the zero field limit, we find large surface potentials whose decay with increasing surfactant concentration resembles the salt-induced screening in aqueous solutions. The amount of surface charge and screening ions in the nonpolar bulk is further characterized via ensemble measurements of the particles' pair interaction energy. In contrast to the behavior reported for systems with *ionic* surfactants, we observe particle charging and a screened Coulomb type interaction both above and below the surfactant's critical micelle concentration.

8:24AM A13.00003 Experimental Studies of the Brownian Diffusion of Boomerang Colloidal Particle in a Confined Geometry, AYAN CHAKRABARTY, FENG WANG, BHUWAN JOSHI, QI-HUO WEI, Kent State University — Recent studies show that the boomerang shaped molecules can form various kinds of liquid crystalline phases. One debated topic related to boomerang molecules is the existence of biaxial nematic liquid crystalline phase. Developing and optical microscopic studies of colloidal systems of boomerang particles would allow us to gain better understanding of orientation ordering and dynamics at "single molecule" level. Here we report the fabrication and experimental studies of the Brownian motion of individual boomerang colloidal particles confined between two glass plates. We used dark-field optical microscopy to directly visualize the Brownian motion of the single colloidal particles in a quasi two dimensional geometry. An EMCCD was used to capture the motion in real time. An indigenously developed imaging processing algorithm based on MatLab program was used to precisely track the position and orientation of the particles with sub-pixel accuracy. The experimental finding of the Brownian diffusion of a single boomerang colloidal particle will be discussed.

8:36AM A13.00004 Effect of Boundary Mobility on the Dynamics of Confined Colloidal Suspensions, GARY L. HUNTER, KAZEM V. EDMOND, ERIC R. WEEKS, Emory University — We use high-speed confocal microscopy to study the influence of boundary mobility on the dynamics of confined colloidal suspensions. Experiments in molecular super-cooled liquids show that confinement can enhance or hinder sample mobility, depending on whether the confining boundary is "soft" (mobile) or "hard" (immobile). We confine suspensions of PMMA microspheres within emulsion droplets of different sizes to examine the consequences of confinement. By changing the viscosity of the external, continuous phase, we also vary the boundary mobility of our samples. In this way, we decouple the effects of confinement and boundary mobility, and draw comparisons between colloidal suspensions and molecular liquids.

8:48AM A13.00005 Observing liquid-gas nucleation in a colloid-polymer solution, RYAN MCGORTY, VINOTHAN N. MANOHARAN, Harvard University, Dept. of Physics — 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 and thermally-responsive colloids we are able to observe the micron-sized nucleating droplets and their fluctuations in three-dimensions. From the droplets' fluctuations we can back out the interfacial tension. Additionally, our three-dimensional imaging technique allows us to capture individual nucleation events and their rate of occurrence. We hope that our data will allow us to better understand nucleation kinetics.

9:00AM A13.00006 Measuring the translational and rotational diffusion of colloidal clusters with digital holographic microscopy, JEROME FUNG, KRISTOPHER ERIC MARTIN, RYAN MCGORTY, DAVID M. KAZ, REBECCA W. PERRY, Harvard University, JOHN A. KELLER, Eastern Nazarene College, GUANGNAN MENG, VINOTHAN N. MANOHARAN, Harvard University — We measure the rotational and translational diffusion coefficients of individual non-spherical colloidal clusters undergoing three-dimensional Brownian motion. We image clusters comprised of spheres approximately 1 μm in diameter using digital holographic microscopy. Fitting the measured holograms to exact electromagnetic scattering calculations allows us to determine cluster positions and orientations with millisecond temporal resolution and ~ 10 nm spatial resolution. For dimers of polystyrene spheres in an aqueous solution, our measurements of the coefficients for rotational diffusion as well as translational diffusion parallel and perpendicular to the dimer axis are consistent with theory. We discuss the extension of this work to non-axisymmetric trimers and potential applications.

9:12AM A13.00007 Density of States of a Two-Dimensional NIPA-Polystyrene Colloidal Crystal¹, MATTHEW GRATALE, PETER YUNKER, KE CHEN, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania — In this work we are interested in how "dopants" affect the vibrational properties of crystals. We study the vibrational density of states of a two-dimensional colloidal crystal consisting of a mixture of hard polystyrene particles and soft NIPA microgel particles. Thus, depending on the particles involved, multiple inter-particle potentials are present in these crystals. The number ratio of hard to soft particles is varied, creating crystals consisting primarily of soft particles doped with hard particles and vice versa. We employ video microscopy to derive the phonon density of states of corresponding "shadow" crystals with the same geometric configuration and interactions as the experimental colloidal system, but absent damping [1,2,3]. Preliminary data reveal low frequency plane-like waves in all crystals, regardless of composition. Participation in higher frequency modes is often enhanced in one species of particles and diminished in the other.

[1] Chen *et al.*, PRL 105, 025501 (2010). [2] Kaya *et al.*, Science 329, 656 (2010). [3] Ghosh *et al.*, PRL 104, 248305 (2010).

¹This work is supported by NSF grant DMR-0804881, MRSEC grant DMR-0520020, and NASA grant NNX08AO0G.

9:24AM A13.00008 Structure and dynamics of confined colloid-polymer mixtures, JACINTA CONRAD, Department of Chemical and Biomolecular Engineering, University of Houston, BINH TRINH, GILDARDO CEBALLOS, Department of Chemical and Biomolecular Engineering, University of Houston — Colloidal processing routes typically require attractive suspensions to be flowed through fine geometries such as microchannels, nozzles, or thin films. To elucidate the effects of confinement on attractive suspensions during processing, we use confocal microscopy to image the structure and dynamics of model colloid-polymer mixtures as a function of confinement dimensionality and thickness, colloid volume fraction, and the strength and range of the attraction. We characterize the phase behavior of the confined suspensions, and find that confinement induces non-uniform structural changes within colloidal gels.

9:36AM A13.00009 Controlling the size distribution of self-assembled colloidal clusters¹, NICHOLAS SCHADE, Harvard Department of Physics, JESSE COLLINS, JONATHAN FAN, MIRANDA HOLMES-CERFON, Harvard SEAS, VINOTHAN MANOHARAN, Harvard Department of Physics — Using a combination of experiment and simulation, we investigate the structures that form when spherical colloidal particles cluster around spheres of different sizes in a binary mixture. We use either oppositely charged particles or particles coated with complementary DNA sequences to form the clusters. Using optical microscopy, we examine the effect of the stoichiometric ratio, the size ratio, and the type of interaction on the distribution of clusters. These parameters serve as useful control mechanisms for the synthesis of nanostructures with tunable properties. For example, a high density of tetrahedral clusters of metallo-dielectric spheres could be used to create a bulk, isotropic metamaterial.

¹We acknowledge support from NSF grant no. ECCS-0709323 as well as the DOE Office of Science Graduate Fellowship Program.

9:48AM A13.00010 Dynamics of interfacial breach by colloidal spheres, DAVID M. KAZ, RYAN MCGORTY, Harvard University, MADHAV MANI, University of California at Santa Barbara, VINOTHAN N. MANOHARAN, Harvard University — We present observations of individual colloidal spheres as they approach and penetrate a flat aqueous interface. Polystyrene spheres with various surface chemistries (sulfate, carboxyl, etc) are brought to the boundary between an oil phase (decane) and an aqueous phase (water+glycerol+NaCl) using radiation pressure from a tightly focused laser. Holographic images are recorded at up to 24,000 frames per second and subsequently compared with Mie-scattering calculations to obtain positional data at a resolution of 5nm in x,y, and z. Typical trajectories consist of an approach to the interface that is dominated by hydrodynamics; a discontinuous jump at the point of penetration (POP); and a very long timescale relaxation that is logarithmic in time. We find that the concentration of salt in the aqueous phase must be above a certain threshold (depending on species) for breach to occur. Well above this threshold, trajectories just prior to the POP are characterized by short-timescale features that are non-monotonic in salt concentration. DLVO type calculations reproduce some aspects of these features, but the non-monotonicity remains mysterious.

10:00AM A13.00011 Sub-diffusion of DNA Coated Particles Near a Complementary DNA Covered Surface¹, LANG FENG, QIN XU, Center for Soft Matter Research, New York University, RUOJIE SHA, NADRIAN SEEMAN, Chemistry Department, New York University, PAUL CHAIKIN, Center for Soft Matter Research, New York University — We have measured the diffusive behavior of micrometer sized colloids in a DNA covered particle-surface system. Near the particle-surface melting temperature of $\sim 45^\circ\text{C}$ we observe conventional diffusion but as temperature is lowered we see a crossover to sub-diffusion over a narrow temperature range. The sub-diffusive behavior is intimately related to the broad distribution of local trapping times. We present a theoretical model which explains the sub-diffusion exponent μ in $\langle R^2(t) \rangle \sim t^\mu$, which ranges from $\mu = 1$ at 44.7°C to $\mu = 0.33$ at 44.1°C . From the distribution of number of DNA bonds we calculate the trapping time distribution and average trapping time. When the measurement time exceeds the average trapping time the system is in equilibrium and exhibits conventional diffusion. When the measurement time is less than the average trapping time the system is not in equilibrium and is sub-diffusive.

¹NASA NNX08AK04G

10:12AM A13.00012 Multiple-Stage Melting and Freezing of Colloidal Crystallites with Short-range Attraction, LIQUAN PEI, Department of Physics, University of Massachusetts Amherst, J.R. SAVAGE, Department of Physics, Cornell University, A.D. DINSMORE, Department of Physics, University of Massachusetts Amherst — We study the dynamics of melting and freezing in a model colloidal system with short-range, temperature tunable attraction. In particular, we mix micron-sized, charge stabilized polystyrene spheres with salt and the surfactant micelles. The micelles induce depletion attraction whose range is less than 2% of the sphere diameter and whose magnitude changes strongly with temperature. We use optical microscopy to record the dynamics of freezing and melting following temperature changes. We use particle tracking algorithms to identify the particles with sub-pixel resolution. For samples with area fraction less than 40%, we have observed that melting and freezing occur in multiple stages, with a metastable liquid phase appearing in both processes. For the freezing sample at area fraction 55%, we have found that the gas droplets are nucleated from high area fraction background. The data also show how nucleation dynamics are affected by the metastable gas-liquid binodal. We are also investigating the role of the second, metastable solid phase in melting and freezing. Our results are relevant to systems where non-equilibrium states may play a role in phase separation.

10:24AM A13.00013 Colloidal aggregation in microgravity by critical Casimir forces, SANDRA VEEN, PETER SCHALL, University of Amsterdam, MARCO POTENZA, MATTEO ALAIMO, University of Milan, STEFANO MAZZONI, European Space Agency, GERARD WEGDAM, University of Amsterdam, VAN DER WAARLS ZEEMAN INSTITUTE, UNIVERSITY OF AMSTERDAM COLLABORATION, OPTICS AND MICROGRAVITY RESEARCH LABORATORY, UNIVERSITY OF MILAN COLLABORATION, PHYSICAL SCIENCE UNIT, EUROPEAN SPACE AGENCY COLLABORATION — We study aggregation and crystal growth of spherical Teflon colloids in binary liquid mixtures in microgravity by the critical Casimir effect. The critical Casimir effect induces interactions between colloids due to the confinement of bulk fluctuations (density or concentration) near the critical point of liquids. The strength and range of the interaction depends on the length scale of these fluctuations which increase as one approaches the critical point. The interaction potential can thus be tuned with temperature. We follow the growth of structures in real time with Near Field Scattering. Measurements are performed in microgravity in order to study pure diffusion limited aggregation, without disturbance by sedimentation or flow.

10:36AM A13.00014 Particle interactions in colloids are revealed in a nonlinear effect in light transmission, JINSUK SONG, DANIEL OU-YANG — Studies on interactions between particles in highly concentrated suspensions are rare because the solutions are opaque and the interpretations from methods such as diffusing wave spectroscopy are often complicated. We propose a simple method of probing particle interactions in the opaque solution by measuring light transmission affected by optically induced particle concentration enhancement. The increase in the particle concentration with the input light intensity depends on the interactions between particles. We demonstrate how this method can be used to determine single particle trapping energy and the virial coefficients in aqueous suspensions of 190 nm polystyrene spheres.

10:48AM A13.00015 Nano-dumbbells pack densely to form birefringent photonic crystals, JASON FORSTER, JIN-GYU PARK, Yale, MANISH MITTAL, University of Delaware, VINODKUMAR SARANATHAN, HEESO NOH, CARL SCHRECK, RICHARD PRUM, COREY O'HERN, HUI CAO, Yale, ERIC FURST, University of Delaware, ERIC DUFRESNE, Yale — Monodisperse spherical colloidal particles robustly self-assemble into crystals at high concentration. We study the self-assembly of polymer nano-dumbbells and find that they crystallize only under strong confinement - in thin films less than three particles thick. On the other hand, external electric fields can readily align dumbbell-shaped particles to make a birefringent suspension. When the electric field is turned off, the dumbbells rapidly lose their orientational order and the birefringence quickly goes away. However, if the solvent is removed with the electric field on, the particles self-assemble into a novel dense crystalline packing hundreds of particles thick. We describe the essential physics of self-assembly of these structures through an interplay of the applied electric field and capillary forces.

Monday, March 21, 2011 11:15AM - 1:51PM –
Session B9 DFD: Nanofluidics D220

11:15AM B9.00001 Message in a bottle: the statistical behavior of nanoparticles in optical confinement¹, H. DANIEL OU-YANG, JOSEPH JUNIO, LIANGCHENG ZHOU, Lehigh University — In an aqueous medium, container surfaces can significantly alter the behavior of suspended nanoparticles. We propose a method to investigate nanoparticle behavior in a boundary-free environment by transiently trapping them with a focused laser beam. While optically confined, as in an optical bottle, these particles are affected by both particle-light and particle-particle interactions. Time-averaged fluorescence imaging produces results in 3D mapping of the nanoparticle concentration in the bottle. We report how we analyze the messages in the bottle, i.e. the statistical behavior of these particles, by using the 3D distributions obtained under both controlled optical and interparticle forces.

¹This project is supported in part by NSF DMR 0923299, Pennsylvania Department of Commerce and Economic Development through the Center for Optical Technologies at Lehigh University and the Pennsylvania Department of Health CURE Formula Funds.

11:27AM B9.00002 Low-frequency dielectric response of a single particle in aqueous suspensions, JINGYU WANG, Physics, Lehigh University, Bethlehem, PA, USA 18015, H. DANIEL OU-YANG, Physics and Bioengineering, Lehigh University, Bethlehem, PA, USA 18015 — α -relaxation, the counterion diffusion in the electric double layer, has been used to describe the anomalous low frequency dielectric dispersion of aqueous suspensions of colloidal particles. A microscopic theory describing this relaxation process proposed by Schwarz, however, has not been investigated systematically. We propose to use a single particle dielectrophoresis (DEP) force spectroscopy to study the relaxation mechanism as a function of particles size, temperature and solvent viscosity. Specifically, we measure the dependence of the DEP crossover frequency force and compare results with predictions by Schwarz.

11:39AM B9.00003 Investigation of MEMS force sensors for nano-scale water measurements¹, SOYOUNG KWON, WONHO JHE, COREY STAMBAUGH, Seoul National University — Nanoscale water formed by capillary condensation has typically been studied by means of an atomic force microscope (AFM). While this approach can provide details about the dynamic visco-elastic properties, it is limited in the type of information that can be measured. Here we propose replacing the fixed sample surface generally used in AFM systems with movable micro-mechanical force sensors (MEMS) fabricated specifically for tapping mode or shear mode. By incorporating a MEMS device we can directly measure the adhesion force, pull-in distance and capillary force of nano confined water while the AFM collects information pertaining to the dynamic visco-elastic properties. In this talk, we will characterize the force measurement in the system and discuss the behavior of the device in the presence of nano-scale water.

¹Work supported NRF of Korea and NSF grant OISE #0853104.

11:51AM B9.00004 Investigation of the Static and Dynamic Mechanical Properties of Nano-scale Water¹, COREY STAMBAUGH, SOYOUNG KWON, WONHO JHE, Seoul National University — The behavior of liquids on the nano-scale has become an area of interest as new fabrication techniques have allowed for increasingly smaller structures to be made. While much work has been done on the interactions forces at liquid and solid interfaces, questions still remain regarding the behavior of nano-scale liquids. By incorporating a micro-electromechanical force sensor (MEMS) into the quartz tuning fork based atomic force microscope (QTF-AFM) probe setup we are able to both manipulate and measure nano-scale water, which in turn provides information beyond the standard AFM approach. Here we look at both the static and dynamic mechanical properties of water formed between the tip of a (QTF-AFM) probe and the polysilicon surface of a MEMS device.

¹Work supported by NSF grant OISE #0853104.

12:03PM B9.00005 Thermophoretic stretching of DNA in polymer nanochannels, JONAS PEDERSEN, LASSE THAMDRUP, HENRIK FLYVBJERG, ANDERS KRISTENSEN, Technical University of Denmark — We demonstrate that thermophoretic forces generated by light-induced local heating can enhance the extension of genomic-length DNA confined in a polymer nanochannel. By temperature control on the micron-scale, bacteriophage T4 DNA is locally stretched to 80% of its contour length, although the cross-section of the nanochannel is as large as 250x250nm². A coarse-grained model of the forces at play captures the DNA-molecule's response to thermophoretic forces with accuracy and precision, and allows for fitting the density profile of the stretched DNA with only a single fit-parameter. The forces involved are relatively strong, because they add up along the molecule. They are measured by using the molecule as an entropic spring balance. Pending a calculation of these forces, this experiment might discriminate between the competing theories for thermophoretic forces.

12:15PM B9.00006 Poisson or not Poisson: Probability distribution of colloidal nanoparticles in an optical trap, YI HU, XUANHONG CHENG, H. DANIEL OU-YANG — In a colloidal suspension of nanoparticles, the presence of an optical trap can exponentially enhance the probability of finding the particles in the vicinity of the trap. Intriguing questions arise regarding whether the probably distribution of particle number in the trap follows Poisson approximation, and if so, what is the upper limit of the trapping energy at which Poisson is followed. To answer these questions, we conduct experiments to determine directly the variance and the mean particle number in the trap at different trapping energies and compare with the predictions of the probability theory.

12:27PM B9.00007 Charging Dynamics of Sub-nanometer Pores, YING LIU, Clemson University, GUANG FENG, JINGSONG HUANG, BOBBY SUMPTER, Oak Ridge National Laboratory, VINCENT MEUNIER, Rensselaer Polytechnic Institute, RUI QIAO, Clemson University — Electrodes featuring sub-nanometer pores can potentially improve the energy density of supercapacitors significantly. However, ions entering such narrow pores often need to pay an energy penalty because part of their solvation shell must be removed. This can potentially limit the charging kinetics of such nanopores. In this work, we investigate the charging dynamics of sub-nanometer pores connected with an electrolyte bath. We quantify the energy barrier for ions to enter 0.82-nm wide slit pores and determine the time constant for charging of the pores using Molecular Dynamics simulations. Strong concentration polarization is found during the charging process and the charging kinetics is much slower than that predicted using the classical equivalent circuit model. The results are rationalized using a modified Poisson-Nernst-Planck model.

12:39PM B9.00008 Statics and Dynamics of Stretched Single DNA Molecules Tug-of-War at Micro-Nanofluidic Interfaces, JIAWEI YEH, Institute of Physics, National Taiwan University, ALESSANDRO TALONI, Tel Aviv University, YENG-LONG CHEN, CHIA-FU CHOU¹, Institute of Physics, Academia Sinica — Understanding single molecule dynamics at micro-nanoscale interfaces has implications to polymer transport in biological processes, device design for single molecule analysis and biotechnological applications. We report our study on single DNA molecules straddling across a nanoslit, bridging two micro-nanofluidic interfaces, for both its tug-of-war behavior and confinement-induced entropic recoiling at varying length and height (h : 30~100 nm) of a nanoslit. From a modified worm-like chain model in the tug-of-war scenario and the scaling analysis in the entropic recoiling process, we demonstrate the entropic recoiling force is essentially constant, given the degree of confinement, irrespective of the DNA length inside the nanoslit and the slit length. The scaling exponents for the entropic force will also be discussed.

¹corresponding author

12:51PM B9.00009 Long time dynamics of single linear and circular ds-DNA confined in sub-100nm nanoslits, PO-KENG LIN, JEN-FANG CHANG, I. STACHIV, CHIA-FU CHOU, Y.-L. CHEN, Institute of Physics, Academia Sinica, Taipei Taiwan — We investigate the role of topological constraints on DNA dynamics in very strong confinement to study the dynamics of nuclear chromosome and DNA viral packaging. Experiments and simulations were carried out to investigate the equilibrium shape and dynamics of the single linear and circular λ -DNA confined in a silicon/glass nanoslit. We measured the chain extension r , shape asphericity A , extensional ($\tau_{||}$) and rotational relaxation time τ_r , and examined the dependence on chain topology as functions of the slit height h (20 ~ 780 nm) and the solvent ionic strength I (0.8 ~ 250 mM). We observed that the shape asphericity increases as h and I decrease as the chain shape becomes anisotropic. Moreover, in sub-Kuhn length confinement, the DNA relaxation time increases with decreasing h in a smooth and broad transition.

1:03PM B9.00010 Heat-Driven Release of a Drug Molecule From Carbon Nanotubes, VITALY CHABAN, OLEG PREZHDO, University of Rochester — Hydrophobicity and ability to absorb light that penetrates through living tissues make carbon nanotubes (CNTs) promising intracellular drug delivery agents. Following insertion of a drug molecule into a CNT, the latter is delivered into a tissue, is heated by near infrared radiation, and releases the drug. In order to assess the feasibility of this scheme, we investigate the rates of energy transfer between CNT, water and the drug molecule, and study the temperature and concentration dependence of the diffusion coefficient of the drug molecule inside CNTs. We use ciprofloxacin (CIP) as a sample drug: direct penetration of CIP through cell membranes is problematic due to its high polarity. The simulations show that a heated CNT rapidly deposits its energy to CIP and water. All estimated timescales for the vibrational energy exchange between CNT, CIP and water are less than 10 ps at 298 K. As the system temperature grows from 278 K to 363 K, the diffusion coefficient of the confined CIP increases 5-7 times, depending on CIP concentration. The diffusion coefficient slightly drops with increasing CIP concentration. This effect is more pronounced at higher temperatures. The simulations support the idea that optical heating of CNTs can assist in releasing encapsulated drugs.

1:15PM B9.00011 Characterization of Nanostructured Silicon Membranes for Control of Molecular Transport, BERNADETA SRIJANTO, SCOTT RETTERER, JASON FOWLKES, MITCHEL DOKTYCZ, Oak Ridge National Laboratory — Fabrication of nanoporous membranes for selective transport of molecular species requires precise engineering at the nanoscale. The membrane permeability can be tuned by controlling the physical structure and the surface chemistry of the pores. We use a combination of electron-beam and optical lithography, along with cryogenic deep reactive ion etching, to fabricate silicon membranes that are physically robust and have uniform pore sizes. Pore sizes are further reduced using plasma enhanced chemical vapor deposition and atomic layer deposition of silicon dioxide onto the membrane surfaces. Integrating nanoporous membranes within a microfluidic network provides a platform for tailoring molecular exchange between microchannels, independent of hydrodynamic effects. In enzymatic reactions, for example, tuning the pores size will allow smaller enzymatic substrates to traverse the membrane at controlled rates while larger enzymes remain spatially separated. Our results from membrane cross-sectioning using focused ion beam milling show that pore sizes can be controlled at dimensions below 10nm. Functional characterization was performed by quantitative fluorescence microscopy to observe the selective transport of molecular species of different sizes.

1:27PM B9.00012 Thermal resistance of thin water films during phase-change, NITIN SHUKLA, NENAD MILJKOVIC, RYAN ENRIGHT, EVELYN N. WANG, Device Research Laboratory, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139 — The thermal resistance of a thin water film during phase-change processes is of interest for fundamental studies and of importance for various engineering systems. In particular, as the thickness of the water film approaches the nanoscale, the thermal resistance across the liquid-vapor interface can contribute significantly to the overall heat transport. In this work, we experimentally investigate the thermal resistance of thin water films during phase change on metallic substrates using transient thermoreflectance (TTR) spectroscopy. This technique offers a novel method to examine heat transport in evaporating liquid films less than a 100 nm in thickness. The understanding gained from this work will aid in the design of high performance phase-change based micro/nanoscale devices.

1:39PM B9.00013 Effect of hydrogen bond cooperativity on the behavior of water, KEVIN STOKELY, Boston University — Four scenarios have been proposed for the low-temperature phase behavior of liquid water, each predicting different thermodynamics. The physical mechanism which leads to each is debated. Moreover, it is still unclear which of the scenarios best describes water, as there is no definitive experimental test. Here we address both open issues within the framework of a microscopic cell model by performing a study combining mean field calculations and Monte Carlo simulations. We show that a common physical mechanism underlies each of the four scenarios, and that two key physical quantities determine which of the four scenarios describes water: (i) the strength of the directional component of the hydrogen bond and (ii) the strength of the cooperative component of the hydrogen bond. The four scenarios may be mapped in the space of these two quantities. We argue that our conclusions are model-independent. Using estimates from experimental data for H bond properties the model predicts that the low-temperature phase diagram of water exhibits a liquid-liquid critical point at positive pressure.

Monday, March 21, 2011 11:15AM - 2:15PM —

Session B13 DFD: Focus Session: Polymer Colloids: Structure, Function, and Dynamics II

11:15AM B13.00001 Predicting long-time Brownian dynamics of ultrasoft colloid suspensions from thermodynamics, MARK POND, The University of Texas at Austin, JEFFREY ERRINGTON, State University of New York at Buffalo, THOMAS TRUSKETT, The University of Texas at Austin — Suspensions of ultrasoft colloids, such as Gaussian-core particles and Hertzian spheres, have received significant research interest due to their reentrant melting behavior and dynamic anomalies. Many of the previous dynamic studies of these systems have focused on molecular dynamics simulations, which by their nature ignores the solvent medium. We have conducted Brownian dynamics simulations of these ultrasoft colloid suspensions to show their long-time dynamic behavior near the reentrant melting transition. In addition, we have developed a novel method for quantitatively and qualitatively predicting the long-time Brownian dynamics of ultrasoft colloidal suspensions from their thermodynamic properties.

11:27AM B13.00002 Development of surfaces repelling negatively buoyant solid particles, CARINA SEMMLER, ALEXANDER ALEXEEV, Georgia Institute of Technology — Using a hybrid computational method that integrates the lattice Boltzmann model for fluid dynamics and the lattice spring model for solids, we examine the motion of negatively buoyant solid microparticles in shear flow near a solid wall decorated with regularly distributed rigid posts. The posts are arranged in a square pattern and tilted relative to the flow direction. We show that when rigid posts are tilted against flow, secondary flows emerge that prevent the deposition of suspended particles on the solid surface. We probe the effect of post geometry on the development of secondary flows and identify the optimal post architecture in terms of the mass of levitated solid particles. Our results are useful for designing anti-fouling surfaces that repel colloidal particles carried by fluid.

11:39AM B13.00003 Microscopic structure of confined colloidal suspensions under shear, XINLIANG XU, STUART RICE, AARON DINNER, James Franck Institute, University of Chicago, XIANG CHENG, ITAI COHEN, Department of Physics, Cornell University — We report a study of driven colloidal suspensions by Stokesian dynamics simulation. The suspension is confined by two parallel plates, and is being driven far away from equilibrium by shearing induced by translation of the parallel plates. The separation of the plates is varied so the suspensions form either a single layer or two layers. Both the structure of the non-equilibrium steady state and the dynamics of the relaxation of the non-equilibrium state back to the equilibrium are examined, at a wide range of shearing strengths (the non-dimensional ratio quantifying the driven motion relative to the Brownian motion of the colloidal particles, the Peclet number is tuned from 0.1 to 100) and packing fractions. We observe string-like structures at low packing fractions and shear-induced crystallization at high fractions. A mechanism is proposed for how hydrodynamic interactions give rise to these structures.

11:51AM B13.00004 Evaporation of Lennard-Jones Fluids, SHENGFENG CHENG, JEREMY LECHMAN, STEVEN PLIMPTON, GARY GRETT, Sandia National Laboratories — Solvent evaporation is a process frequently used to disperse particles in a bulk material or at a substrate. The local order and packing of particles can be controlled by controlling the evaporation rate. The first step to fully understand this complicated process is to understand the evaporation process of pure liquid at the microscopic scale. We have carried out large scale molecular dynamics simulations to study the evaporation of Lennard-Jones (LJ) fluids composed of monomers, dimers, or trimers. For LJ monomers in contact with a vacuum, the evaporation rate is found to be very high with significant evaporative cooling and an accompanying density gradient in the liquid domain near the liquid/vapor interface. Increasing the chain length to just dimers significantly reduces the evaporation rate. The velocity distributions of evaporated monomers are measured and compared to a kinetic theory and their dependence on the evaporation conditions is discussed. For nanoparticle suspensions, the nanoparticles order at the surface, which causes the evaporation to significantly slow down.

12:03PM B13.00005 Rotational and Translational Diffusion of PMMA Colloidal Clusters, HYUN JOO PARK, MARK T. ELSESSER, New York University, KAZEM V. EDMOND, Emory University, DAVID J. PINE, New York University, NEW YORK UNIVERSITY COLLABORATION, EMORY UNIVERSITY COLLABORATION — Colloidal clusters, 3-7 μm in size, are a good model system for various 2D and 3D structures depending on the aggregation number, N . We measure the translational and rotational diffusion of individual dyed PMMA clusters of dimers and trimers using high speed confocal scanning microscopy and particle tracking. We report measurements of the rotational and translational diffusion coefficients (and their ratios) as a function of volume fraction.

12:15PM B13.00006 A diversity of binary colloidal crystals using DNA-directed interactions, JOHN CROCKER, MARIE UNG, W. BEN ROGERS, RAYNALDO SCARLETT, TALID SINNO, University of Pennsylvania — DNA is the premier tool for directing the controlled self-assembly of nanoscopic and microscopic objects. The interactions between microspheres due to the hybridization of DNA strands grafted to their surface have been measured and can be modeled in detail, using well-known polymer physics and DNA thermodynamics. Knowledge of the potential, in turn, enables the exploration of the complex phase diagram and self-assembly kinetics in simulation. In experiment, at high densities of long grafted DNA strands, and temperatures where the binding is reversible, these systems readily form colloidal crystals having a diverse range of symmetries. For interactions that favor alloying between two same-sized colloidal species, our experimental observations compare favorably to a simulation framework that predicts the equilibrium phase behavior, crystal growth kinetics and solid-solid transitions. We will discuss the crystallography of the novel alloy structures formed and address how particle size and heterogeneity affect nucleation and growth rates.

12:27PM B13.00007 Correlating Structural and Spectral Fluctuations in a Lasing Colloidal Suspension, JASON W. MERRILL, Yale University, Department of Physics, HUI CAO, Yale University, Departments of Physics and Applied Physics, ERIC R. DUFRESNE, Yale University, Departments of Mechanical Engineering, Physics, Chemical Engineering, and Cell Biology — When multiply scattering media with optical gain are optically pumped above a critical threshold, they emit coherent radiation in many spectral lines. This phenomenon is known as random lasing. The wavelengths of these spectral lines depend sensitively on the spatial distribution of scatterers, but this relationship has only just begun to be explored. We study the time and frequency domain statistics of random laser spectra emitted from dense colloidal suspensions doped with laser dye with an eye toward using this information as a probe of the underlying colloid dynamics.

12:39PM B13.00008 Smart colloidosomes with tunable permeability and a dissolution trigger, ADRIANA SAN MIGUEL, JAN SCRIMGEOUR, JENNIFER CURTIS, SVEN BEHRENS, Georgia Tech — Self-assembly of colloidal particles in the liquid interface of double emulsion droplets can be used to fabricate “colloidosome” microcapsules, which have great potential as vehicles for the controlled delivery of drugs or other cargoes. Here we present a novel class of aqueous core colloidosomes that combine the benefit of low capsule permeability (good cargo retention) with the option of a stimulus-triggered fast release in a target environment. Complete or partial dissolution of the capsule walls in response to a mild pH change is achieved in each case through the use of responsive particles made from polymers with pH-switchable solubility. We demonstrate three methods of controlling the capsule permeability prior to release while maintaining the intended response to the release trigger.

12:51PM B13.00009 A theoretical study of colloidal forces near an amphiphilic polymer brush, JIANZHONG WU, University of California, Riverside — Polymer-based “non-stick” coatings are promising as the next generation of effective, environmentally-friendly marine antifouling systems that minimize nonspecific adsorption of extracellular polymeric substances (EPS). However, design and development of such systems are impeded by the poor knowledge of polymer-mediated interactions of biomacromolecules with the protected substrate. In this work, a polymer density functional theory (DFT) is used to predict the potential of mean force between spherical biomacromolecules and amphiphilic copolymer brushes within a coarse-grained model that captures essential nonspecific interactions such as the molecular excluded volume effects and the hydrophobic energies. The relevance of theoretical results for practical control of the EPS adsorption is discussed in terms of the efficiency of different brush configurations to prevent biofouling. It is shown that the most effective antifouling surface may be accomplished by using amphiphilic brushes with a long hydrophilic backbone and a hydrophobic end at moderate grafting density.

1:03PM B13.00010 Phase transition of colloidal particles on curved surfaces, GUANGNAN MENG, JAYSON PAULOSE, DAVID NELSON, Department of Physics, Harvard University, VINOTHAN MANOHARAN, Department of Physics and School of Engineering and Applied Sciences, Harvard University — Defects and disclinations have to appear in crystalline domains on a curved surface with non-zero Gaussian curvature. These geometrical frustrations can qualitatively change the physics of phase transition. We encapsulate micron sized polystyrene (PS) colloidal particles within emulsion droplets and use nanometer sized polyNIPAM hydrogel particles to introduce depletion attraction between PS particle and interface, as well as between PS particles. We use this experimental model system and confocal microscopy to study phase transitions on curved surfaces. We will present both experimental phenomena and theoretical analysis.

1:15PM B13.00011 Dielectric effects in self-assembly of binary colloid mixtures, ERIK LUIJTEN, KIPTON BARROS¹, Northwestern University — Colloidal self-assembly is often controlled by electrostatic interactions. The solvent and colloids typically have different dielectric constants, thereby inducing polarization charge at the colloid surfaces. A shortcoming of previous simulations of charged colloids with implicit solvent is the neglect of the effective many-body interactions resulting from such dielectric effects. We study colloidal self-assembly using a method that properly accounts for polarization charge. In simulations of weakly charged colloids with large size asymmetry, we find that dielectric effects modify the pair correlation function in a nontrivial way and at low temperatures alter the observed crystal phase.

¹Currently at Los Alamos National Laboratory.

1:27PM B13.00012 Formation of three-dimensional colloidal nanoparticle supercrystals and probing the formation kinetics, IRVING HERMAN, Columbia University, CHENGUANG LU, AUSTIN AKEY, Columbia University — A multiple solvent system consisting of colloidal nanoparticles in several solvents of gradually decreasing vapor pressures was investigated in the self assembly of hundred-layer thick colloidal nanoparticle superlattices in lithographically defined capillaries. Such a solvent system allows a very slow and tunable drying rate of solvents, which, together with the microfluidic flow into the capillaries, leads to the controllable formation of large, single crystalline 3D nanoparticle supercrystals. The underlying mechanism of superlattice formation was investigated via the drying rates for nanoparticle assembly for solvent systems of specific compositions. This technique generates single-crystalline 3D supercrystals of \sim micrometer size at spatially controlled locations, and large chunks (up to 40 μ m by 40 μ m by 5 μ m) of single crystalline supercrystals on a flat Si substrate. The ordered nature of the structures formed was probed by high-resolution SEM and small angle x-ray scattering. In-situ x-ray scattering reveals the formation kinetics of the transition of nanoparticle assemblies from amorphous to ordered. This technique is versatile and has been applied to various types and sizes of colloidal nanocrystals, including those composed of CdSe, Au, PbS and Fe₃O₄.

1:39PM B13.00013 Nanoparticle-induced self-assembly of functionalized tetrapods, DANIEL W. SINKOVITS, University of Illinois at Urbana-Champaign, ERIK LUIJTEN, Northwestern University — Recent advances in synthesis have made it possible to create monodisperse particles with well-defined shapes. In particular, tetrapods have been fabricated in a wide range of well-controlled dimensions and have been functionalized in several different ways. We present Monte Carlo simulations of the self-assembly of functionalized tetrapods. We consider how the addition of charged spherical nanoparticles provides another means to control the self-assembled structure. In addition, we report the results of simulations of planar tripods confined to two dimensions and demonstrate that highly regular structures can be achieved without functionalization, through nanoparticle-mediated depletion interactions.

1:51PM B13.00014 A “diffusing diffusivity” model of “anomalous yet Brownian” diffusion of colloidal particles, MYKYTA V. CHUBYNSKY, GARY W. SLATER, Department of Physics, University of Ottawa, Canada — “Anomalous yet Brownian” diffusion of colloidal beads, with a mean-square displacement (MSD) exactly linear in time (as in simple Fickian diffusion) but an exponential (rather than Gaussian) displacement distribution (DD) at short times for large displacements, has been reported recently by Granick’s group [1] in several systems. We argue that a strictly linear MSD with a non-Gaussian DD is a universal feature of systems with “diffusivity memory” (a particle diffusing faster is likely to keep diffusing faster for some time), but without “direction memory” (a jump in a particular direction does not change the probability of subsequent jumps in that direction). We consider a series of toy models reproducing this behavior in which a particle undergoes regular diffusion, but its diffusivity itself performs a (perhaps biased) random walk. The DD is strictly exponential at short times when the diffusivity distribution itself is exponential, but an exponential remains a good fit for a variety of diffusivity distributions.

[1] Wang et al., PNAS 106 (2009) 15160.

2:03PM B13.00015 Reentrant and Isostructural Transitions in the Cluster-Crystal Forming GEM-4, KAI ZHANG, PATRICK CHARBONNEAU, Duke University, BIANCA MLADEK, University of Cambridge — Systems governed by soft, bounded, purely repulsive interactions show two possible equilibrium behaviors under compression: reentrant melting, as in the Gaussian core model (GCM), or clustering, as in the penetrable sphere model (PSM). The generalized exponential model of power 4 (GEM-4), which is the intermedia of the GCM and PSM with a simple isotropic pair interaction $u(r) \sim e^{-r^4}$, is thought to belong to the second family and was indeed found to form clusters at sufficiently high densities at high temperatures. Here, we present the low-temperature behavior of GEM-4 through Monte Carlo simulations using a specially developed free energy integration scheme. We find the phase behavior to be hybrid between the GCM and the PSM limits, showing a surprisingly rich phase behavior in spite of the simplicity of the interaction form. For instance, S-shaped doubly reentrant phase sequences and evidence of a cascade of critical isostructural transitions between crystals of different average lattice site occupancy are observed. The possible annihilation of lattice sites and accompanying clustering moreover leads to an unusual softening upon compression, which suggest that these materials may have interesting mechanical properties. We discuss possible experimental realizations and challenges of this class of materials.

Monday, March 21, 2011 2:30PM - 5:30PM –
Session D9 DFD: Patterns, Nonlinear Dynamics followed by General Fluid Dynamics D220

2:30PM D9.00001 Rayleigh Bénard Convection-A Case Study on Pattern Formation, HIRA SIDDIQUI, RUDOLF FRIEDRICH, WWU Muenster, Germany — Spiral turbulence in Rayleigh-Benard convection is studied numerically in the framework of generalized Swift-Hohenberg equations. The model equation consist of an order parameter equation for the temperature field coupled to an equation for the mean flow field. In contrast to the earlier work, nonlinearities in the dynamics of the mean flow are retained leading to a two dimensional Navier-Stokes equation coupled to a Swift-Hohenberg equation. We present the numerical investigations of nonlinear effects due to the interaction of nonlinear two dimensional flows and the pattern forming process.

2:42PM D9.00002 A simple approach to localized convection, H. PLEINER, Max Planck Inst. for Polymer Research, Germany, M.G. CLERC, Univ. de Chile, Santiago de Chile, J. MARTINEZ-MARDONES, Pont. Univ. Católica de Valparaíso, Chile, L.M. PEREZ, Dep. Ingeniería Metalúrgica, Univ. de Santiago, Chile, D. LAROZE, Max Planck Institute for Polymer Research, Mainz and Inst. de Alta Investigación, Univ. de Tarapaca, Arica, Chile — Localized structures can be found in many different (dissipative) driven systems [1], an example being stationary and traveling convection structures in the thermal instability of binary fluids. Here, the special localized structure is a convective state between two quiescent, conductive ones, and can be interpreted as a pinning phenomenon close to a stationary sub-critical bifurcation. Generally, localized structures are described by using higher dimensional, complex amplitude or phenomenological prototype (e.g. Swift-Hohenberg) equations or by direct numerical integration of the hydrodynamic equations. Here we show, using the binary mixture convection in porous media as an example, that the analytically derived one-dimensional amplitude equation amended by non-adiabatic (non-resonant) terms important close to convection fronts, well describes localized convection states, in particular the slanted homoclinic bifurcation diagrams.

[1] O. Descalzi, M. Clerc, S. Residori, and G. Assanto (Eds.), *Localized States in Physics: Solitons and Patterns*, Springer, 2011.

2:54PM D9.00003 The dynamics of cracks in torn thin sheets, YOSSI COHEN, ITAMAR PROCACCIA, Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel — The stress field near the tip of a crack due to a mode III shear tearing of a thin plate of elastic material has a universal form but with a non-universal amplitude known as the Stress Intensity Factor. All the non-universal aspects of the stress distribution are collected in the Stress Intensity Factor which depends on everything, including the crack length, the boundary conditions and the history of the loads that drive the crack evolution. Although the equations of elasticity for thin plates are well known, there remains the question of selection of a path for a propagating crack. We invoke a generalization of the principle of local symmetry to provide a criterion for path selection and demonstrate the qualitative agreement of our results with the experimental findings. We also analyze the nature of the singularity at the crack tip with and without the nonlinear elastic contributions. Finally we present an exact analytic results for the stress intensity factor to the linear approximation for the crack developing in thin sheets.

3:06PM D9.00004 Chaotic Plume-Like Bursts in Rimming Flows, GABRIEL SEIDEN, VICTOR STEINBERG, Weizmann Institute of Science — We report a detailed experimental investigation of chaotic, plume-like bursts observed in rimming flows of polymer solutions within a partially filled horizontal cylinder. In particular, we investigate the attractive interaction between adjacent plumes and the effect of rotation rate and polymer concentration on the statistics of these unique bursts. A comparison is also made between the Newtonian and non-Newtonian cases.

3:18PM D9.00005 Cracks formation during blood drop evaporation, BENJAMIN SOBAC, DAVID BRUTIN, Université de Provence, UNIVERSITÉ DE PROVENCE TEAM — We firstly presented the pattern formation occurring when drops of whole blood desiccate in a recent publication [1]. The phenomena presented evidence to involve lots of physical field such as surface chemistry, haematology, fluid mechanics, heat transfer, colloids science... All these mechanisms are acting together and produce an axisymmetric and reproducible pattern. Dried cellular components are segregated and deposited by a capillary flow. During the evaporation, the system is slowly drying and cracks when stresses are too important leading to the final pattern observed. In this presentation, we will present the mechanisms involved in the formation of crack patterns. The phenomenon presented here with red blood cells as the main colloids involved is very similar to the drying of drop of nanoparticles [2]. We will explain the common point and the differences encountered.

[1] D. Brutin, B. Sobac, B. Loquet and J. Sampol, *Pattern formation in drying drops of blood*, *Journal of Fluid Mechanics*, underpress, 2010.

[2] L. Pauchard, B. Abou, K. Sekimoto, *Influence of Mechanical Properties of Nanoparticles on Macrocrack Formation*, *Langmuir*, 25(12), 6672-6677, 2009.

3:30PM D9.00006 ABSTRACT WITHDRAWN —

3:42PM D9.00007 Pattern formation and coarsening in crystalline membranes, DANIEL A. VEGA, ALDO D. PEZZUTTI, Dep. de Física- IFISUR- Universidad Nacional del Sur - CONICET — We study through a Brazovskii-Helfrich Hamiltonian the process of defect formation, annealing and coarsening of two dimensional crystalline membranes. In good agreement with the cosmological model of Kibble and Zurek, proposed to determine the density of topological defects at the onset of a symmetry breaking phase transition, we found that the collision of orientationally uncorrelated domains produces a structure of grains with an average density of topological defects controlled by the temperature of the quench. The strain field of the dislocations and disclinations generated during the phase separation process can induce the buckling of the membrane, slowing down the Lifshitz-Safran mechanism of coarsening observed in flat systems.

3:54PM D9.00008 Pattern formation in ternary lipid membranes with composition-deformation coupling, MATTHEW DEMERS, Northwestern University Department of Applied Mathematics, FRANCISCO SOLIS, MONICA OLVERA DE LA CRUZ, Northwestern University Department of Materials Science — We study patterns formed in three-component lipid membranes, where composition is coupled to shape via differences in spontaneous curvature. The system is examined in the strong segregation regime. System morphology is determined by the competition of bending energy, surface tension, and line tension. We will present the phase behavior as determined by numerical minimization, as well as analytic solutions for select cases.

4:06PM D9.00009 Supercavitating flow past an elastic curvilinear hydrofoil¹, YURI ANTIPOV, Louisiana State University — A nonlinear inverse fluid-structure interaction problem is considered. The obstacle is a curvilinear elastic hydrofoil, and the cavity formed behind is modeled according to the single-spiral-vortex model by Tulin. First, the model for a rigid polygonal supercavitating hydrofoil is solved by the method of conformal mappings. The mapping function is expressed through the solutions of two Riemann-Hilbert problems. To identify the vertices of the polygon where the jets break away from the foil, the Brillouin-Villat separation condition is applied. The unknown parameters of the conformal mapping are computed on solving a system of transcendental equations. Next, by increasing the number of vertices of a regular N -polygon, the cavitation problem for a circular arc is solved, pressure on the foil is defined, and a boundary-value problem for a thin shell subject to normal loading is stated. The elastic problem is solved exactly for an arc with clamped ends, and the new hydrofoil profile is determined. Finally, a new cavitation problem for the deformed foil is stated and solved. Numerical experiments reveals the presence of two thin partial cavities near the foil ends.

¹This work was funded by NSF through grant DMS0707724.

4:18PM D9.00010 Drag calculations using the inviscid Euler equations alone, GALEN GISLER, PGP/University of Oslo — Recently Hoffman and Johnson¹ have proposed a new resolution of d'Alembert's Paradox, the problem that inviscid potential flow predicts zero drag on a body, in contrast to observations. They reject the commonly accepted resolution, that drag results from the very thin viscous boundary layer between the no-slip condition on the surface of the body and the free-flowing fluid. Instead they argue that drag results from turbulence in the body's wake, even if free-slip is assumed. They used a finite-volume code to verify their conclusions. While their calculations look promising, and offer prospects for calculation of rather more complex flows at modest resolution, it is desirable to perform independent verification. I will present independent tests of the Hoffman-Johnson resolution using a finite-volume Euler-equation code, studying the dependence of the inferred drag on meshing style and resolution.

[1] Johan Hoffman and Claes Johnson, *J. Math. Fl. Dyn.* 12, 321-334 (2010).

4:30PM D9.00011 Dynamics of induced dipole ER fluid: a continuous energetic approach, JIANWEI ZHANG, WENFENG LI, JIAXI LI, Dept. of Physics, Tongji University, Shanghai, China — We studied dynamics of Electrorheological (ER) fluid by continuum induced dipole fluid method [1]. We found that the velocity profile of ER fluid increases in high shear-rate region and solid particles are separated from colloid in high electric field. These findings demonstrated the breakdown of Bingham fluid model under high shear-rate and high electric field. Our continuum approach describes ER fluid's behaviors under most conditions. We also found that the shift of maximum shear stress under different electric field follows the same trend as that of the maximum static stress. This indicates that the static and dynamic stresses are both dominated by the same energetic process. A connection between micro-particles' structures and macro-dynamic properties under varying conditions is established by our continuum method. Our studies probe the physics of induced dipole ER fluid.

[1] Jianwei Zhang, Xiuqing Gong, Chun Liu, Weijia Wen, and Ping Sheng, Physical Review Letters 101, 194503, 2008.

4:42PM D9.00012 Velocity fluctuations in steadily sedimenting suspensions, K. VIJAY KUMAR¹, SRIRAM RAMASWAMY, CCMT, Department of Physics, Indian Institute of Science, Bangalore 560012 — The simplest model of a homogeneous suspension steadily sedimenting under gravity at low Reynolds number indicates that the velocity fluctuations should diverge with the system size. This is, however, not seen in experiments. We improve on a previously described coarse-grained model proposed for this problem by identifying certain crucial missing terms in the equations of motion. These terms are allowed by symmetry considerations and can be generated by a mechanism which is natural in the dynamics of low Reynolds number sedimentation. A dynamical renormalization group calculation of our model leads to the conclusion that these extra terms are always relevant. If these terms are stabilizing, this suggests a natural mechanism for suppressing fluctuations in sedimenting suspensions. We analyze the properties of the critical point where these extra terms vanish.

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4:54PM D9.00013 Stabilization of toroidal droplets using viscoelastic media, EKAPOP PAIRAM, ALBERTO FERNANDEZ-NIEVES, School of Physics / Georgia Tech Team — We inject a viscous liquid through a needle into another rotating viscous liquid to generate toroidal droplets. These droplets are unstable and undergo a transformation into spherical droplets driven by surface tension: They either break ala Rayleigh-Plateau or grow fatter to become a single spherical droplet depending on the aspect ratio of the torus. By replacing the outer phase with a viscoelastic fluid with a non-zero yield stress we can stabilize these and other non-zero genus droplets. We will examine this stabilization mechanism and present criteria to effectively prevent the break-up of these droplets.

5:06PM D9.00014 Iron chemistry at aqueous interfaces by near edge X-ray spectroscopy¹, DAVID VAKNIN, WENJIE WANG, ALEX TRAVESSET, Ames Laboratory, and Department of Physics, Iowa State University, Ames, Iowa 50011, IVAN KUZMENKO, X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439 — Employing synchrotron X-ray absorption near-edge spectroscopy (XANES) combined with X-ray fluorescence (XF) and reflectivity (XR) techniques, we monitor the state of ferrous and ferric iron as it binds to charged carboxylic and phosphate groups. By subphase pH manipulation, arachidic acid and dihexadecyl phosphate monolayers can provide a range of surface charge density from nearly charge-neutral to a fully charged monolayer to which iron ions are attracted from solutions. Analysis of our results from fluorescence show that the driving forces attracting Fe³⁺ and Fe²⁺ to the interface originate from chemical interactions and electrostatic, respectively. XANES shows that the electronic and geometric structure of iron complexes at interface are different from those in the bulk. Moreover, the XANES results demonstrate that valence state and bonding of the interfacially bound Fe³⁺ and Fe²⁺ are practically indistinguishable. This, we argue, is due to the versatility of iron ions in behaving as electron acceptors (Fe³⁺) or as donors (Fe²⁺).

¹Supported by the Office of BES, U.S. Department of Energy Cont. No. DE-AC02-07CH11358.

5:18PM D9.00015 Interfacial microrheology in viscoelastic membranes, GOPAL SUBEDI, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — Prior studies on interfaces using microrheology have typically been applied to interfaces with only a surface viscosity component and not an elastic one. We are extending the application of interfacial microrheology to viscoelastic lipid monolayers. We use a DPPC and cholesterol lipid monolayer in a Langmuir trough as a model system. The Langmuir trough gives us the flexibility to control the concentration and thus the phase of the monolayer. The microrheology technique allows us to measure the rheology at specific concentrations or in situations as the concentration is changed. The microrheology technique employs video microscopy to record the diffusive motion of micron size spheres placed at the interface. Since the diffusive motion of the microspheres is dominated by the interfacial rheology of the monolayer, the recorded motions of the microspheres are used to infer the rheological properties of the interface. We hope to extend our understanding of viscoelastic interfaces with the study.

Monday, March 21, 2011 2:30PM - 5:30PM –

Session D42 DFD: Colloids Theory & Computation, Emulsions, and Foams A302/303

2:30PM D42.00001 Liquid loss from foams with low water content, MICHAEL CONROY, JUSTIN TAYLOR, JOHN FARLEY, JAMES FLEMING, RAMAGOPAL ANANTH, Naval Research Laboratory — The liquid content of a foam can be significantly affected by liquid loss (drainage), a process that occurs both during and after the foam fills a space. We develop a theoretical model to describe liquid loss and evolution of average liquid volume fraction over time for advancing and static foams. We also perform bench-scale drainage experiments on foams with low water content. The theoretical model shows a constant drainage rate during the filling process which decays exponentially after a static column is formed. The measured loss of liquid is found to be in good agreement with the theoretical predictions. We find that drainage is greatly affected by the time scale for filling a space with foam. Significant effects on drainage are also found by varying bubble size, foam column height, and initial liquid content. The study indicates that drainage behavior can substantially deviate from that described by free-drainage theories, which assume that drainage initiates from a foam of static height.

2:42PM D42.00002 Molecular Dynamics Study of the Foam Stability of a Mixed Surfactant System with and without Calcium Ions, XIAOZHEN YANG, WENHONG YANG, Institute of Chemistry, CAS, INSTITUTE OF CHEMISTRY, CAS TEAM — Foam stability performance of a mixture surfactant system with and without calcium ions, including linear alkylbenzene sulfonate (LAS) and sodium dodecyl sulfate (SDS), has been studied by molecular dynamics. Microscopic interaction analysis reveals that the fraction of free calcium ions, X_f , in film system indicates the extent of the foam stabilities when X_f is in different calcium ion zones. In the system without ions, we found the variable of the surfactant tail mass out of water film, W , is indicator of foam stability. Performance of the mixture system predicted here was supported by experiments.

2:54PM D42.00003 Structural Properties of a Sheared Dense Emulsion¹, S.K. DUTTA, E.D. KNOWLTON, D.L. BLAIR, Department of Physics, Georgetown University — The flow of a compressed emulsion above its yield point can be described by a velocity profile in addition to a rearrangement of individual droplets on top of this time averaged motion. Using a confocal microscope, we have tracked the droplets of an oil-in-water emulsion as they are sheared in a rheometer. When the applied stress is large, the velocity profile shows a nearly affine deformation, while there is strong strain localization close to yield. The crossover between these two behaviors occurs at higher shear rates as the volume fraction of the droplets is increased. At shorter length scales, rearrangement events are heterogeneously distributed, reflecting the disordered packing of the emulsion droplets. This characterization is a step towards linking bulk viscoelastic properties to local structural relaxation as the system leaves the jammed state.

¹This work is funded by the NSF through Grant DMR 0847490.

3:06PM D42.00004 Janus and Gemini Nanoplates, ZHENGDONG CHENG, ANDRES MEJIA, YA-WEN CHANG, PENG HE, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77840, AGUSTIN DIAZ, ABRAHAM CLEARFIELD, Department of Chemistry, Texas A&M University, College Station, TX 77842 — Janus particles were used to make stable Pickering emulsions (emulsions stabilized by particles). Here we demonstrated a novel method to produce high aspect ratio Janus plates with atomic thickness. Gemini plates with only the edges functionalized are also fabricated. These novel nanoplates are observed to have super surface activity. Most importantly, these particles overcome the two *opposite* effects in the stabilization of Pickering emulsions using spherical particles: stabilization requires particles as small as possible; but smaller particles are easy to escape the interface due to Brownian motion since the adsorption energy to the oil-water interface is proportional to the diameter of the spheres. Our nanoplates have a *large* aspect ratio due to the extremely thin thickness, which offers extraordinary stability to the liquid film between two emulsions to prevent coalescence. In the meantime, their large lateral surface area offers strong adsorption energy at the oil-water interface.

3:18PM D42.00005 Control over the number, size, and type of inner drops inside a double emulsion, LAURA ADAMS, YUANJIN ZHAO, ANDERSON SHUM, DAVID WEITZ, Harvard University — The formation of monodisperse double emulsions, drops inside of drops, has revealed a rich range of configurations not possible without the precise control of microfluidics. Yet-to-date, development of double emulsions with a controlled number of two different inner drops has not emerged. Here we demonstrate exquisite control over the number, size and type of inner drops encapsulated inside a double emulsion. These are fabricated using glass capillary devices implemented with a dual bore injection tube. We will show our latest results and discuss the scientific and technological opportunities made possible by these stable binary configurations.

3:30PM D42.00006 Yielding and Shear Induced Structure Formation in Emulsions with Attractive Interactions, ZHEN SHAO, AJAY NEGI, CHINEDUM OSUJI, Yale University, OSUJI LAB TEAM — The yielding behavior of colloidal suspensions is a strong function of inter-particle interactions. Recent results [Pham et al. 2006, 2008] indicate that attractive colloidal glasses display a two-step yielding due to inter-particle bond rupture followed by particle cage escape. From this perspective, we examine the yielding behavior of an oil-in-water emulsion system with attractive interactions using dynamic bulk rheology. In strain sweep experiments, after a limited linear regime, the system yields with a pronounced bump in the viscous modulus, a sharp decrease in the elastic modulus and a crossover between the two. The yielding response is marked by bond-breaking at low volume fractions and bond-breaking accompanied by cage escape above a critical concentration. An increase in the complex modulus is observed at yet higher strains (>100%), with both the elastic and viscous components showing small frequency dependent peaks. The onset, peak strains and peak stress display different dependences on volume fraction. We speculate that this display is due to the formation of shear induced structures at high strains and advance a simple model for this behavior.

3:42PM D42.00007 Force Network in a 2D Frictionless Emulsion Model System, KENNETH W. DESMOND, PEARL YOUNG, DANDAN CHEN, ERIC R. WEEKS, Emory University — We confine oil-in-water emulsion droplets between two parallel plates to create a quasi-two-dimensional model system to study the jamming transition. This model system is analogous to granular photoelastic disks with the exception that there is no static friction between our droplets. To study the jamming transition we compress the droplets in small increments and investigate how the force network evolves with increasing area fraction, where the forces are measured using a calibration technique we have developed. The forces in our system are spatial heterogeneous with a probability distribution that is similar to that found for photoelastic disks. We also find that the probability distribution of the forces narrows with area fraction, and that the correlation length of the largest forces is only few particle diameters.

3:54PM D42.00008 New activated dynamical regimes in dense suspensions of attractive uniaxial colloids, RUI ZHANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — Our microscopic theory of cooperative translational-rotational activated glassy dynamics of hard uniaxial particles [PRE,80,011502(2009); JCP,133,104902(2010)] is extended to treat short range attractions. For small aspect ratio dicolloids, a plastic glass (PG) state exists for weak attractions, but is destroyed beyond a critical attraction strength resulting in a new dynamic triple point (fluid, PG, gel), and two novel re-entrant behaviors: PG-fluid-gel, and repulsive glass(RG)-PG-gel. A new mixed “glass-gel” state also emerges characterized by center-of-mass and rotational angle localization parameters of intermediate magnitude. At high volume fractions, increasing attraction transforms the RG to an attractive glass (AG) characterized by a dynamic free energy surface with a gel-like localization state but a glass-like saddle point, and a non-monotonic variation of relaxation time and diffusion constant. AG dynamics is of a 2-step nature where physical bonds first break followed by hopping over a glass-like barrier. At high attractions a sharp crossover from a gel to AG with increasing volume fraction is predicted. As the particle aspect ratio grows, the PG state is destroyed, and translational motion becomes increasingly more important for escaping dynamical traps.

4:06PM D42.00009 A new analysis methodology for the motion of self-propelled particles and its application, YOUNG-MOO BYUN, PAUL LAMMERT, VINCENT CRESPI, Penn State University — The self-propelled particle (SPP) on the microscale in the solution is a growing field of study, which has a potential to be used for nanomedicine and nanorobots. However, little detailed quantitative analysis on the motion of the SPP has been performed so far because its self-propelled motion is strongly coupled to Brownian motion, which makes the extraction of intrinsic propulsion mechanisms problematic, leading to inconsistent conclusions. Here, we present a novel way to decompose the motion of the SPP into self-propelled and Brownian components; accurate values for self-propulsion speed and diffusion coefficients of the SPP are obtained for the first time. Then, we apply our analysis methodology to ostensible chemotaxis of SPP, and reveal the actual (non-chemotactic) mechanism of the phenomenon, demonstrating that our analysis methodology is a powerful and reliable tool.

4:18PM D42.00010 Diffraction effects on optical trapping of small particles, RACHAEL HARPER, ALEX LEVINE, University of California, Los Angeles — Geometric ray optics is an elegant and computationally efficient means of numerically calculating the forces on particles of arbitrary shape due to their interaction with a beam of light. This method is limited to the regime in which the particle is much larger than the wavelength of light. Ashkin's pioneering work [1] on force exerted by a laser trap on a spherical dielectric particle relies on this geometric optics limit. In current experiments, however, the size of the trapped particles can be comparable to the wavelength of the trapping radiation field. In this talk, we discuss the corrections to ray-tracing-based calculations of the laser trapping forces due to diffraction effects. Specifically, we compare the momentum transfer from a uniform beam of light to hollow dielectric cylindrical shells obtained from two different calculations using: (i) ray-tracing and (ii) the full physical optics formulation. By changing the radii of the inner and outer edges of the hollow cylinder with respect to the wavelength of light we determine the limits of validity of the ray-tracing solution. In the limit in which the radius of the inner cylinder is comparable to the wavelength radiation we show that the corrected momentum transfer is smaller than that predicted by geometric optics. We attribute this result to the reduction in the scattering force on the cylinder due to diffraction effects not accounted for in the geometric optics formalism. [1] A Ashkin, Biophys. J., 61, 569 (1992).

4:30PM D42.00011 Capillary Interactions among Spherical Particles at a Curved Liquid Interface, CHUAN ZENG, University of Massachusetts Amherst, FABIAN BRAU, Physique Theorique, Universite de Mons, BENNY DAVIDOVITCH, ANTHONY D. DINSMORE, University of Massachusetts Amherst — Colloidal particles tend to adsorb on liquid interfaces, where in-plane interactions can arise from a variety of mechanisms. We focus on capillary interactions induced by the curvature of the liquid interface, where particles were assumed to have a constant Young-Laplace contact angle at the three-phase contact line. Whereas spherical particles can adsorb on flat or spherical interfaces without deforming the interface, adsorption on a cylindrical interface deforms the interface because of the lack of azimuthal symmetry around the contact line. We present an analytical model of the interfacial shape and energy upon adsorption of a single particle as well as the interaction between two particles. Based on our result on a cylindrical interface, we propose a general formula for the force on a particle on a curved interface. This study provides an important step toward understanding the interactions among interfacial particles when the interface is distorted by an external field. We acknowledge support from the NSF-supported MRSEC on Polymers at UMass (DMR- 0820506) and NSF CBET-0967620.

4:42PM D42.00012 Slow relaxations of individual colloidal spheres following the breach of a fluid interface, MADHAV MANI, KITP & UCSB Physics, DAVID M. KAZ, RYAN MCGORTY, VINOTHAN N. MANOHARAN, Harvard University — Although the equilibrium state of a micron sized spherical particle at an interface is well understood, the dynamics associated with the approach to equilibrium is not. Recent high-resolution experiments from the Manoharan Lab (Ref: David M. Kaz's Talk) have shown that the dynamics are richer than expected. Subsequent to the initiation of a contact-line at a fluid interface the dynamics towards equilibrium are much slower than predicted by a hydrodynamic theory and the center of mass of the particle appears to follow a logarithmic law in time. We propose the importance of thermally agitated interactions between the contact-line and physical/chemical defects that pin the contact-line locally, thereby leading to an enhancement of the overall dissipation. We deduce that the interface must remain flat during this dynamic process and derive a force-velocity relation, which agrees with both the slow velocities and the logarithmic law. This surprisingly slow approach to equilibrium has significant consequences for processes where interactions between colloids and interfaces are present.

4:54PM D42.00013 Using Micron-Sized Ellipsoids as a New Tool for Microrheology, DAVID KILGORE, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — It is a well-established principle that the viscosity of a fluid can be calculated by observing the diffusion of microspheres, provided the diameter of the microspheres is known. We are developing a microrheology technique using ellipsoids, where the rheology can be measured without prior knowledge of the length and width of the ellipsoid. The advantage of using ellipsoids is that their asymmetry allows for the diffusion to be decomposed into two translational motions and one rotational motion. For each of these diffusive motions, we can measure a diffusion constant and relate the constant to the three unknowns: the length and width of the ellipsoid, and the viscosity. By measuring the three diffusion constants, we can determine the three unknowns. To verify this technique, we produce ellipsoids in the lab and suspend them in a viscous solution for three-dimensional imaging of the diffusion with a confocal microscope. We are able to get good agreement between the microrheological measurements and macroscopic viscosity measurements.

5:06PM D42.00014 Inferring elastic properties in colloidal solids: artifacts of a restricted observation window, ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — Recently, it has been shown how to extract information about the effective elasticity in colloidal solids, granular packings, *etc.*, using two point displacement correlations as obtained in, *e.g.*, optical microscopy experiments or computer simulations. At its core, this technique relies on the observation that, within the harmonic approximation, the Hamiltonian, H , is the inverse of the elastic response function, G , defined over the whole domain of the elastic body. However, most experiments (and even most simulations) have access to G only over some restricted sub-domain of the experimental system. Here, we study restricted observation domains of various size and dimensionality in face centered cubic (fcc) crystals of various size using a pseudo-analytic approach in which G is obtained analytically and is inverted numerically on a compact sub-domain to obtain the projected Hamiltonian, \tilde{H} . We show that the effective plane-wave energy, $E_k = \langle \psi_k | \tilde{H} | \psi_k \rangle$, for either a [111] or [100] planar subdomain has an unusual dispersion, $E \sim k$, rather than the familiar $E \sim k^2$ and motivate this observation from continuum considerations. We also show how this leads to an anomaly in the density of states of \tilde{H} .

5:18PM D42.00015 Enhancing tracer diffusivity by tuning interparticle interactions and solvation shell structure, JAMES CARMER, GAURAV GOEL, TOM TRUSKETT, University of Texas at Austin Chemical Engineering — Using computer simulations, we explore how tuning the tracer-solvent interactions affects the dynamics of a tracer particle. Optimizing the tracer particle contribution to excess entropy results in significant increases in tracer particle diffusivity. We also observe increases in dynamics while increasing the effective particle size. These changes are investigated at various densities and particle size ratios.

Tuesday, March 22, 2011 8:00AM - 11:00AM —
Session H9 DFD: Colloids: Experimental D220

8:00AM H9.00001 Universality in the delayed failure of colloidal gels, JORIS SPRAKEL, DAVID WEITZ, Harvard University — The mechanical failure of heterogeneous solids is not always instantaneous with the application of a load, but can be significantly delayed. We use colloidal gels, a prototypic heterogeneous material, to unravel the microscopic mechanisms behind this delayed failure. A universal behavior is revealed; the delay time depends only on the magnitude of the applied stress not on its origin. Whether the gel succumbs to internal tension, gravitational compression or shear stresses, the behavior can be quantitatively explained using a generalized bond-rupture model that describes the microscopic events triggering macroscopic failure.

8:12AM H9.00002 Glassy dynamics of 2D colloid crystals in a random pinning potential¹, SUNGCHEOL KIM, ALEXANDROS PERTSINIDIS², XINSHENG LING, Brown University — Recently, we have demonstrated that a monolayer charged colloidal crystal confined to a rough charged surface provides a realization of the Larkin-Ovchinnikov random-pinning model in two dimensions [1]. The statics of the system is found to agree with Larkin's prediction of balkanization into small ordered domains. However, the dynamics are in disagreement with the collective creep model. Detailed analysis of the particle trajectories suggest that collective creep is preempted by channel flow. We also find that the velocity response to a step-like driving force shows a stretched exponential behavior similar to that found in structural glasses. Here, we provide a detailed analysis of this process.

[1] A. Pertsinidis and X.S. Ling PRL **100** 028303 (2008)

¹This research was supported by the NFS-DMR.

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8:24AM H9.00003 Field-driven pattern formation of charged particles in nonpolar solvent, TINA LIN, SHMUEL RUBINSTEIN, DAVID WEITZ, Harvard University — We combine microfluidics and high-speed imaging to investigate transport dynamics of charged colloidal particles in a nonpolar solvent as the polarity of an external electric field is switched periodically. Immediately following a switch, particles which were initially all packed against one electrode move towards the opposite electrode in an unstable manner; instead of remaining uniform, the particle front develops undulations. This results in a heterogeneous deposition of particles on the electrode wall. For a range of wait times between switches, we find that the particles localize at exceptionally well-defined periodic modes and we offer a simple physical model to account for this pattern formation.

8:36AM H9.00004 Colloids with magnetic patches: synthesis and self-assembly, STEFANO SACANNA, NYU, LAURA ROSSI, Utrecht University, WILLIAM IRVINE, DAVID PINE, NYU — We developed a new class of colloidal particles that programmably and reversibly self-assemble into well-defined clusters by virtue of “magnetic patches” carrying a permanent magnetic dipole moment. The resulting clusters form spontaneously in a zero external field, and their geometry is entirely determined by the interplay between magnetic, steric, and electrostatic interactions. Imposing an external magnetic field enables the clusters to unbind or change their geometry allowing, in principle, to create materials with tunable structural arrangements.

8:48AM H9.00005 Melting Dynamics of Colloidal Thin Films on Patterned Substrates, JOHN MERGO, School of Applied and Engineering Physics, Cornell University, JOHN SAVAGE, Department of Physics, Cornell University, ITAI COHEN, Department of Physics, Cornell University — We present results of experiments on the melting dynamics of colloidal crystals formed on patterned substrates. Our system consists of micron-sized colloidal particles and a tunable short-range attractive depletion interaction that can be controlled by small temperature changes. We investigate the melting rates of crystalline islands that form on substrates with square and hexagonal symmetry. We find that crystals with square symmetry melt significantly slower than those with hexagonal symmetry despite the fact that particles at the edge of the hexagonal crystal are on average bound more strongly than those at the edge of a square crystal. We find that the symmetry of the substrate affects the ability of particles to diffuse away from a melting crystal, and these differences in single-particle diffusion rates account for the difference in melting rates.

9:00AM H9.00006 Dynamics of Transient Vorticity Aligned Structures in Attractive Colloidal Suspensions, AJAY NEGI, Yale University, MICHELLE BEBRIN, McGill University, CHINEDUM OSUJI, Yale University — Shear rate jumps from high to low flow rates in an attractive colloidal suspension of carbon black particles in a non-polar solvent result in the formation of transient log-like structures aligned in the vorticity direction. Optical microscopy in situ with bulk rheology shows that the appearance of these aggregates is attended by an increase in the suspension viscosity. The viscosity shows a peak and then gradually recedes with passage of time under flow in concordance with the disappearance of the log-like structures. The time at which the viscosity reaches its maximum scales inversely with the shear rate applied to the system. This emergence of the peak in viscosity appears to be controlled by a critical strain and rescaling in these terms produces a common response across several different shear rates. Alteration of the attraction strength between particles by the addition of surfactant severely inhibits the structure formation. We present a simple model to account for these observations.

9:12AM H9.00007 Two-dimensional Fibonacci spiral optical thermal ratchets, KE XIAO, DAVID GRIER, Center for Soft Matter Research at New York University — A novel two-dimensional optical thermal ratchet has been implemented with holographic optical trapping arrays structured as the “Fibonacci spiral” for diffusing colloidal particles. Periodically rotating the optical trapping array by an angle in a three-step cycle yields a two-dimensional time-varying optical landscape that acts either as (1) a deterministic pump when traps are closely dispersed in space, whose induced radial and azimuthal fluxes can be quantitatively mapped out according to the geometry of Fibonacci spiral, or else as (2) an optical thermal ratchet when traps are widely dispersed, whose transport property depends on the competition between the temporal evolution in optical landscapes and Brownian particles' diffusivity. The Fibonacci ratchet displays independent flux reversals in both the radial and azimuthal directions as a function of the cycle frequency and the inter-trap separation.

9:24AM H9.00008 Using shear to assemble colloidal strings, ITAI COHEN, XIANG CHENG, Dept. of Physics, Cornell University — Sheared colloidal suspensions exhibit various fascinating phases under the influence of hydrodynamic, interparticle and thermal interactions. These shear-induced phases have been intensively studied for suspensions well above the crystalline threshold, but remain relatively unexplored for amorphous suspensions. Here, we report a novel string phase in less concentrated colloidal suspensions under shear, where particles assemble into long strings normal to the plane of shear. This finding contradicts previous numerical results that predict the formation of particle strings along the shear velocity direction. We systematically investigate how the phase depends on the shear rates, the confinement of shear plates, and the volume fractions of samples. We demonstrate the relation between the string phase of low volume fraction samples and the shear-induced crystallization of high volume fraction samples. A simple mechanism for the formation of this novel phase is suggested.

9:36AM H9.00009 Biomembrane-mediated control of like-charge colloidal attraction, MAUNTA MANANDHAR, YUPENG KONG, RAGHUVeer PARTHASARATHY, Department of Physics and Material Science Institute, The University of Oregon — The nature of attractions observed between like-charged colloidal particles near a confining wall is still mysterious, due in part to the lack of experimental systems with tunable inter-particle interactions. Biomembranes are appealing candidates for colloidal functionalization, enabling access to electrostatic and chemical properties that influence inter-particle relations. Previous optical-trap based examinations of lipid membrane functionalized particles revealed a surprising linear relationship between the magnitude of the attractive pair potential and the particle charge in presence of a wall of constant charge density. Here, using lipid membranes to also functionalize the confining wall, thereby controlling its charge density, we find a non-linear relationship between inter-particle attraction and charge. Our results highlight the role of substrate-induced fields in controlling pair interactions between colloidal microparticles.

9:48AM H9.00010 Colloidal Gas-Liquid Condensation induced by the Critical Casimir Effect, DUC NGUYEN, SUZANNE FABER, GERARD H. WEGDAM, PETER SCHALL, University of Amsterdam — We explore a new temperature control over colloidal phase formation by using the Critical Casimir effect. This effect allows direct control over particle interactions via temperature-dependent solvent fluctuations: In analogy to the confinement of fluctuations of the electromagnetic field between two dielectrics (quantum mechanical Casimir effect), the confinement of fluctuations of a critical solvent leads to an attraction between surfaces that are immersed in this solvent. This allows exquisite temperature control over the interactions of colloidal particles that are suspended in this critical solvent. We show that this temperature control allows us to “freeze” a dilute colloidal gas into a dense colloidal liquid, and a crystalline solid. By using confocal microscopy, we follow these phase transitions directly in real space, and we measure the particle pair potential. We show that we can quantitatively account for the gas-liquid condensation by using Van der Waals theory. We study the growth of colloidal liquid droplets by following the mean droplet radius $\langle R \rangle$ with dynamic light scattering. We find $\langle R \rangle \sim t^{1/2}$ and $\langle R \rangle \sim t^{1/3}$ indicating that the droplets form by nucleation, followed by diffusion limited growth.

10:00AM H9.00011 Comparison of different analysis techniques in inline holographic video microscopy, FOOK CHIONG CHEONG, New York University — Holographic video microscope can be analyzed on a frame-by-frame basis to track individual colloidal particles' three-dimensional motions with nanometer resolution. In this work, we compare the performance of two complementary analysis techniques, one based on fitting to the exact Lorenz-Mie theory and the other based on phenomenological interpretation of the scattered light field reconstructed with Rayleigh-Sommerfeld back-propagation. Although Lorenz-Mie tracking provides more information and is inherently more precise, Rayleigh-Sommerfeld reconstruction is faster and more general.

10:12AM H9.00012 Dynamics of colloidal particles in ice, MELISSA SPANNUTH, S.G.J. MOCHRIE, Yale University, S.S.L. PEPPIN, Oxford University, J.S. WETTLAUFER, Yale University — Solidification of the solvent phase of a colloidal suspension occurs in many natural and technological settings and is becoming a popular technique for creating microporous structures and composite materials. During freezing, regions of high particle density can form as particles are rejected from the growing solid and guided into a variety of macroscopic morphologies. The particles in the high density regions form an amorphous colloidal solid that deforms in response to internal and external stresses. Using X-ray Photon Correlation Spectroscopy, we studied this deformation for silica particles in polycrystalline ice. We found that the particles in the high density regions underwent ballistic motion coupled with a non-exponential decay of the intensity autocorrelation function (ACF) that transitions from a stretched to a compressed exponential with increasing scattering vector q . While ballistic motion and a compressed exponential decay of the ACF is common, the coupling with a stretched exponential decay is very rare and a transition with increasing q has not previously been reported. We explain this behavior in terms of ice grain boundary migration.

10:24AM H9.00013 Imaging the microscopic structure of shear thinning and thickening colloidal suspensions, XIANG CHENG, Dept of Physics, Cornell University, JONATHAN MCCOY, Department of Physics and Astronomy, Colby College, JACOB ISRAELACHVILI, Dept. of Chemical Engineering, University of California, Santa Barbara, ITAI COHEN, Dept. of Physics, Cornell University — The viscosity of colloidal suspensions varies by orders of magnitude depending on how quickly they are sheared. Such non-Newtonian behavior arises from the arrangement of suspended particles and their mutual interactions. Although numerical simulations and various scattering experiments have revealed much about the local and average suspension structures, particle dynamics at mesoscopic length scales, where non-Newtonian behaviors are believed to originate, are still poorly understood. Here, by combining fast confocal microscopy with simultaneous rheological measurements, we systematically investigate changes in suspension structure over a range of length scales, as the suspension transitions through regimes with different rheological signatures. Our measurements bridge previous simulation and scattering results, and unambiguously show that shear thinning is coupled to particle layering, that shear thickening is decoupled from suspension order-to-disorder transitions, and that there exists a novel phase where particles self-assemble into strings oriented normal to the plane of shear.

10:36AM H9.00014 Cubic crystals from cubic colloids, LAURA ROSSI, Van't Hoff Laboratory, Utrecht University, STEFANO SACANNA, WILLIAM IRVINE, PAUL CHAIKIN, DAVID PINE, Center for Soft Matter Research, New York University, ALBERT PHILIPSE, Van't Hoff Laboratory, Utrecht University — We have studied the crystallization behavior of colloidal cubes by means of tunable depletion interactions. The colloidal system consists of novel micron-sized cubic particles prepared by silica deposition on hematite templates and various non-adsorbing water-soluble polymers as depletion agents. We show that under certain conditions the cubes can self-organize into crystals with a simple cubic symmetry, which is set by the size of the depletant. The dynamic of crystal nucleation and growth is investigated monitoring the samples in time by optical microscopy. Furthermore, by using temperature sensitive microgel particles as depletant it is possible to fine tune depletion interactions as to induce crystal melting. Assisting crystallization with an alternating electric field improves the uniformity of the cubic pattern allowing the preparation of macroscopic (almost defect-free) crystals that show visible Bragg colors.

10:48AM H9.00015 Spin-coating of rapidly dried colloidal suspensions: model and experiments¹, MAXIMILIANO GIULIANI, University of Guelph, WENCESLAO GONZÁLEZ-VIÑAS, University of Navarra, ANAND YETHIRAJ, Memorial University of Newfoundland — The study of the formation of colloidal crystals has been a very active field in recent years. The spin-coating technique has proven to be a highly reproducible process to form large area colloidal crystals. Here, we present recent results on spin-coating of rapidly dried colloidal suspension. We show that the dynamics observed can be represented by an extension of classical Emslie model to highly volatile fluids. We obtained this extension while maintaining the explicit solution for the temporal evolution of the fluid thickness. We observed that the dynamics can be separated in two regimes: one dominated by non-evaporative effects and a second dominated by evaporative effects. The transition between these two dynamical regimes corresponds well with the transition between two symmetries observed during the fluid phase (six and four-fold). Similarly, the quality of the deposited structure is also well correlated to the relative strength of the capillary forces with respect to the viscous ones.

¹Support from NSERC, and MEC (FIS2008-01126).

Tuesday, March 22, 2011 11:15AM - 2:15PM – Session J9 DFD: Liquid Crystals: Nematics, Lyotropics and Vesicles D220

11:15AM J9.00001 Dynamics of chiral liquid-crystal films driven by water transport¹, JONATHAN V. SELINGER, LENA M. LOPATINA, Liquid Crystal Institute, Kent State University — In previous experimental and theoretical research, Tabe and Yokoyama investigated Langmuir monolayers of chiral molecules on the surface of water, and found that evaporation of water induces collective precession of the molecular orientation [1]. More recently, they have found a similar effect in freely suspended films of chiral smectic liquid crystals, but with one new feature: the molecular rotation is accompanied by large-scale flow of the molecules, indicating a strong coupling between orientation and flow. To model the coupled rotation and flow driven by water transport, we construct the Lagrangian and Rayleigh dissipation function appropriate for a film in the smectic-A or smectic-C phase, derive the equations of motion, and solve these equations in geometries corresponding to the experiments. In particular, we calculate the flow patterns in terms of the viscosity coefficients of the liquid-crystal films, in order to understand the mechanisms that control this dynamic behavior. The theoretical predictions are compared with experimental results, and with related work on granular materials [2].

[1] Y. Tabe and H. Yokoyama, *Nature Mat.* 2, 806 (2003).

[2] J.-C. Tsai, F. Ye, J. Rodriguez, J. P. Gollub, and T. C. Lubensky, *Phys. Rev. Lett.* 94, 214301 (2005).

¹This work was supported by NSF Grant DMR-0605889.

11:27AM J9.00002 Linear aggregation and liquid-crystalline order: comparison of Monte Carlo simulation and analytic theory, TATIANA KURIBOVA, University of Colorado, M.D. BETTERTON, MATTHEW A. GLASER, University of Colorado at Boulder — Many soft-matter and biophysical systems are composed of monomers that reversibly assemble into rod-like aggregates. The aggregates can then order into liquid-crystal phases if the density is high enough, and liquid-crystal ordering promotes increased growth of aggregates. Systems that display coupled aggregation and liquid-crystal ordering include wormlike micelles, chromonic liquid crystals, DNA and RNA, and protein polymers and fibrils. Coarse-grained molecular models that capture key features of coupled aggregation and liquid-crystal ordering common to many different systems are lacking; in particular, the roles of monomer aspect ratio and aggregate flexibility are not well understood. We study a system of sticky cylinders that interact primarily by hard-core interactions but can stack and bind end to end. We use Monte Carlo simulations and analytic theory. We present results for several different cylinder aspect ratios and a range of end-to-end binding energies. The phase diagrams are qualitatively similar to those of chromonic liquid crystals, with an isotropic-nematic-columnar triple point. Our analytic theory shows improvement compared to previous theory in quantitatively predicting the I-N transition for relatively stiff aggregates, but requires a better treatment of aggregate flexibility.

11:39AM J9.00003 Modeling the Kerr effect in polymer-disordered liquid crystals¹, LENA M. LOPATINA, JONATHAN V. SELINGER, Liquid Crystal Institute, Kent State University — In the Kerr effect, an electric field applied to an optically isotropic material induces orientational order and hence induces optical birefringence. Recently, many investigators have used the Kerr effect to develop liquid-crystal displays and other electro-optic devices that can operate at high speed and with no need for aligning substrates. This application requires a large and fairly temperature-independent Kerr coefficient. One approach to achieve this goal is by using liquid-crystal blue phases, perhaps with polymer stabilization. As an alternative approach, D.-K. Yang has suggested using a nematic phase within a disordered polymer network. This structure would be disordered and optically isotropic in the absence of a field, but it would develop order and birefringence under an applied field. To assess this approach, we perform Monte Carlo simulations of a nematic liquid crystal in a disordered polymer network, and calculate the response to an applied field. We compare the results with analytic studies of liquid crystals under quenched disorder and with experiments.

¹This work was supported by NSF Grant DMR-0605889.

11:51AM J9.00004 A nonlocal model of inhomogeneous nematic liquid crystals, PETER PALFFY-MUHORAY, Liquid Crystal Institute - KSU, XIAOYU ZHENG, Dept. of Mathematical Sciences - KSU, ROLAND ENNIS, Pressco Technology Inc. Cleveland, OH — The free energy cost of spatial inhomogeneities in nematic liquid crystals is usually described in terms of gradients of the director field or of the order parameter tensor. The origins of such gradient expansions are not clear; they can also lead to ill-posedness of the variational problem of minimizing the free energy. We propose a simple nonlocal form of the single particle potential from which the free energy may be constructed. Our model reduces to the Maier-Saupe form for homogenous systems, but describes inhomogeneous systems in general. We demonstrate the validity of the model by using it to describe the electric field induced Freedericksz transition. We discuss the connection between our non-local model and gradient expansions.

12:03PM J9.00005 Freely Suspended Nematic Films¹, WILDER IGLESIAS, JEFFREY CHOI, ELIZABETH K. MANN, ANTAL JAKLI, Kent State University — Using one of the most commonly studied synthetic molecule, 4-Cyano-4'-pentylbiphenyl (5CB), we were able to pull freely suspended membranes of different thicknesses into circular frames of up to 20mm diameter. Films pulled this way were distorted using a speaker, while a laser light was shone onto them for studying the far field reflection and learn about resonant frequency modes and subtract valuable information about the viscoelastic terms that hold the membrane stable.

¹This work was supported by NFS, grant 0907055.

12:15PM J9.00006 Fluctuation Modes of a Bent-Core Nematic Liquid Crystal¹, MADHABI MAJUMDAR, S. CHAKRABORTY, B. SENYUK, O.D. LAVRETOVICH, JAMES T. GLEESON, ANTAL JAKLI, SAMUEL SPRUNT, Kent State University — We present a dynamic light scattering study of the bent-core nematic liquid crystal compound *DT6Py6E6*. We utilize a "dark" scattering geometry, which allows us to search for fluctuation modes that are not purely associated with the uniaxial director. Indeed, we observe two modes (hydrodynamic and non-hydrodynamic) in addition to the expected twist-bend director mode. We present a model for the additional modes based on fluctuations of the biaxial order parameter, which leads to an estimate of 10-100 nm for the correlation length associated with these fluctuations.

¹Acknowledgement: DOE DE-SC0001412 and NSF DMR-0606160.

12:27PM J9.00007 Three dielectric constants and orientation order parameters in nematic mesophases¹, HYUNG GUEN YOON, SEUNG YEON JEONG, SATYENDRA KUMAR, Kent State University, MIN SANG PARK, JUNG OK PARK, M. SRINIVASARAO, Georgia Institute of Technology, SUNG TAE SHIN, LCD R&D Center, Samsung Electronics Corp. — Temperature dependence of the three components ϵ_1 , ϵ_2 , and ϵ_3 of dielectric constant and orientation order parameters in the nematic phase of mesogens with rod, banana, and zero-order dendritic shape were measured using the in-plane and vertical switching geometries, and micro-Raman technique. Results on the well-known uniaxial (N_u) nematogens, E7 and 5CB, revealed two components $\epsilon_1 = \epsilon_{||}$ and $\epsilon_2 = \epsilon_3 = \epsilon_{\perp}$, as expected. The three dielectric constants were different for two azo substituted (A131 and A103) and an oxadiazole based (ODBP-Ph-C12) bent core mesogens, and a Ge core tetrapode. In some cases, two of the components became the same indicating a loss of biaxiality at temperatures coinciding with the previously reported N_u to biaxial nematic transition. This interpretation is substantiated by micro-Raman measurements of the uniaxial and biaxial nematic order parameters.

¹Supported by the US Department of Energy, Basic Energy Sciences grant ER46572 and by Samsung Electronics Corporation.

12:39PM J9.00008 The interplay between fluctuations in physical structure and power consumption in electroconvecting liquid crystals, JOHN CRESSMAN, ZRINKA GREGURIC, TYRUS BERRY, TIMOTHY SAUER, George Mason University — We will present results from experiments performed on the nematic liquid crystal MBBA. We have made simultaneous measurements of the optical patterns formed in the weakly-driven electroconvective state, as well as the electrical power consumed by the sample. By performing a dimensionality reduction on the optical data we identify the dominant modes in the system and go on to elucidate the role of these modes in the measured power fluctuations. We will conclude by discussing these results in the context of the free energy derived by de Gennes for nematic liquid crystals.

12:51PM J9.00009 Magneto-optical technique for detecting biaxial nematic phase¹, TANYA OSTAPENKO, J.T. GLEESON, S.N. SPRUNT, A. JAKLI, Kent State University — There have been numerous attempts to find a thermotropic liquid crystal that exhibits a biaxial phase. There have been findings of biaxial order in bent-core nematic liquid crystals; however, there are recent reports that call this into question. One reason for this discrepancy is the difficulty in unambiguously identifying the biaxiality. Based on a previously described electro-optical technique, we have developed a technique that uses magnetic field, thus widening its application to any bent-core nematic material. The field orients the uniaxial director along the optical path length, and we search for birefringence perpendicular to this direction. We expect one of two situations to occur: if the material is uniaxial, the induced phase difference will decrease asymptotically to zero as the field increases. However, if the material is biaxial, the induced phase will extrapolate to a non-zero value. Results on one calamitic liquid crystal show that this method yields the expected result, namely the lack of biaxial nematic phase. We also tested several bent-core nematic liquid crystals and found that none of these materials exhibits a biaxial nematic phase.

¹This work was supported by the NSF (DMR-0606160). Work performed at NHMFL supported by the NSF, the State of Florida and the DOE.

1:03PM J9.00010 Nonlinear electrophoresis in nematics: Flows and effects of salts, ISRAEL LAZO-MARTINEZ, OLEG D. LAVRENTOVICH, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University — Electrophoresis (EP) in a nematic liquid crystal (LC) is dramatically different from its isotropic counterpart, as the EP velocity has a component that is quadratic in the applied electric field [1]. Unlike the regular EP velocity that is linear in the field, this component does not vanish in an ac field with a zero time average, which makes the LC EP attractive for applications where the steady flows are needed. EP propulsion is caused by distortion of the LC orientation around the particles that break the fore-aft (or left-right) symmetry, leading towards an imbalance of field-induced flows around the particles. We visualize the flows and measure the EP velocity by recording 3D trajectories of passive tracers suspended in the LC under the fluorescent confocal polarizing microscope. We demonstrate that doping the LC with organic salts increases the EP velocities. The work was supported by NSF DMR 0906751.

[1] O. D. Lavrentovich, I. Lazo, O. P. Pishnyak, *Nature* 467, 947-950 (2010).

1:15PM J9.00011 Anisotropic Stokes Drag and Dynamic Lift on Cylindrical Colloids in a Nematic Liquid Crystal, JOEL ROVNER, CLAYTON LAPOINTE, DANIEL REICH, ROBERT LEHENY, Johns Hopkins University — Unlike isotropic fluids, nematic liquid crystals exhibit a complex assortment of hydrodynamic properties that can strongly depend on the director field and local boundary conditions set by inclusions. To understand further these characteristics, measurements were taken of the Stokes drag on magnetic nanowires suspended in nematic 4-cyano-4'-pentybiphenyl (5CB). Effective drag viscosities for wires moving perpendicular and parallel to the nematic director were measured and were found to differ by factors of approximately 0.88 to 2.4, depending on the wire orientation and surface anchoring. Additionally, a lift force was observed when wires were forced at an oblique angle to the director resulting in motion divergent from the line of force. The lift was greater for wires with homeotropic anchoring and smaller for wires with longitudinal anchoring, suggesting that the lift force can act as a mechanism for sorting colloidal particles according to their surface chemistry.

1:27PM J9.00012 Morphology and Rheology of the Liquid Crystal-Colloid Composites, LU ZOU, CHANJOONG KIM, Liquid Crystal Institute, Kent State University — Liquid crystal (LC)-colloid composites form aggregates and are arrested in various network structures. We study viscoelastic properties and three-dimensional structure of nematic LC-colloid composites using fluorescence confocal polarized rheoscope and fluorescence microscope. We observe various morphological transformations of the composites when we cool them down below T_{NI} from the high temperature isotropic phase. We find that colloidal particles are self-organized to ferny structures, and that the morphological characteristics of the ferny structures depend on the applied shear rates, the cooling rate, the particle volume fraction and the particle size. This study may offer a new route to form novel colloidal structures using anisotropic fluid, which could not be obtained from isotropic suspensions.

1:39PM J9.00013 Structural Reorganization of Liquid Crystals Revealed by Fast Scanning Calorimeter¹, DONGSHAN ZHOU, JING JIANG, XIAOLIANG WANG, GI XUE, Nanjing University — Liquid crystal glass of 4-Cyano-4'-octylbiphenyl is obtained by rapid cooling with rates over 2000 Kelvin per second (K/s) on the chip calorimeter. The glass can crystallize easily upon heated above its glass transition temperature. Depending on the prior cooling rate and annealing history thereafter, melting-structural reorganization-remelting behavior similar to that of semicrystalline polymer can be observed during subsequent heating. The complex melting behavior is attributed to the transformation of metastable crystal forms formed during annealing or heating induced cold crystallization. Increasing the heating rate (>15000 K/s) can suppress the transformation and, additionally, enables us to capture the multiple N-I transition. This implies the coexistence of two different types of nematic states. To avoid above complex structural reorganization, one can anneal the sample at 260K for 2 seconds to get the stable crystal form.

¹The work is financially supported by the National Science Foundation of China (NSFC: 20504014, 20874045, 50533020, 20774041) and National Basic Research Program of China, No 2007CB925101.

1:51PM J9.00014 Parity breaking in nematic tactoids of lyotropic chromonic liquid crystals¹, LUANA TORTORA, OLEG D. LAVRENTOVICH, Liquid Crystal Institute, Kent State University — In many colloidal systems, an orientationally ordered nematic phase emerges from the isotropic melt in the form of spindle-like birefringent tactoids. In cases studied so far, the tactoids always reveal a mirror-symmetric non-chiral structure, even when the building units are chiral, as in the case of tobacco mosaic virus [1] and fd virus [2]. We report on parity breaking in the nematic tactoids formed in molecularly non-chiral polymer-crowded solutions of lyotropic chromonic liquid crystals. The effect is manifested by twist of the director and optical activity. Fluorescent confocal polarizing microscopy reveals that the tactoids nucleate at boundaries of cells. We explain the chirality induction by the effect of geometrical anchoring [3] and by increase of the splay elastic constant in condensed nematic regions of crowded solutions.

[1] J. D. Bernal and I. Fankuchen, *J. Gen. Physiol.* **25**, 111 (1941);

[2] Z. Dogic, *Phys. Rev. Lett.* **91**, 165701 (2003);

[3] O.D. Lavrentovich, *Phys. Rev. A* **46**, R722 (1992)

¹NSF DMR MWN 0710544

2:03PM J9.00015 Orientational order and defect structures on curved surfaces¹, SUBAS DHAKAL, Northwestern University, FRANCISCO J. SOLIS, Arizona State University, MONICA OLVERA DE LA CRUZ, Northwestern University — We study the topological defects in a nematic liquid crystal confined to a surface. Using Monte Carlo simulations, we investigate how the position and number of defects depend on the interaction strength, the shape of the surface and other physical parameters. On a spherical surface, we find that the interaction changes the location of four +1/2 defects initially sitting on a great circle of the sphere to the vertices of a tetrahedron. In deformed spheres, we observe the coalescence of defects into two single +1 defects.

¹We acknowledge the support of the NERC, which is a EFRC funded DOE Office of Science under Award DE-SC0000989.

Tuesday, March 22, 2011 11:15AM - 2:15PM –
Session J44 DPOLY DFD: Focus Session: Kinetic Control of Solution Assemblies A309

11:15AM J44.00001 Helical Assembly of Janus Particles, JONATHAN WHITMER, Department of Physics, University of Illinois at Urbana-Champaign, QIAN CHEN, SHAN JIANG, SUNG CHUL BAE, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, ERIK LUIJTEN, Department of Materials Science and Engineering and Department of Engineering Sciences and Applied Mathematics, Northwestern University — Amphiphilic Janus particles, which have hydrophobic and hydrophilic hemispheres, assemble into a variety of clusters depending on salt concentration and particle volume fraction. At low salt concentration, repulsion due to surface charges keeps cluster sizes small, whereas at higher salt concentrations beautiful elongated helices of tetrahedra emerge. We demonstrate that the emergence of these helical structures is a nonequilibrium effect, and that kinetic selection drives formation of polytetrahedral shapes relative to polyhedral shapes which are entropically more favorable.

11:27AM J44.00002 Nucleation of Nanoparticle Superclusters from Solution¹, SIDDIQUE J. KHAN, C.M. SORENSEN, A. CHAKRABARTI, Dept. of Physics, Kansas State University — Colloids of surface ligated nanoparticles (NP) often act as solutions with the NP displaying reversible temperature and solvent dependent solubility. In many cases when the nanoparticles are highly uniform, the precipitating solid is a two- or three-dimensional superlattice of the nanoparticles. Thus there is strong analogy to the phase behavior of molecular solutions, and it is reasonable to ask what controls the phase behavior of nanoparticle solutions and what is the nature of nucleation and growth of the insoluble phase? We have recently developed [1] a phenomenological model for the effective interaction potential between two ligated gold nanoparticles. In the current work, we carry out Brownian Dynamics simulations using this NP-NP interaction potential. We will report results from our simulations for both dynamics and shape of pre-nucleating and post-nucleating superclusters.

[1] S.J. Khan, F. Pierce, C.M. Sorensen and A. Chakrabarti, *Langmuir*, 25, 13861 (2009).

¹Supported by NSF NIRT grant CTS0609318.

11:39AM J44.00003 Directing the self-assembly of polyhedral silver nanocrystals, MICHAEL GRUENWALD, University of California at Berkeley, JOEL HENZIE, ASAPH WIDMER-COOPER, PHILLIP GEISSLER, PEIDONG YANG — Self-assembly of nanocrystals with complex shapes requires precise control of nanoscale interactions and driving forces. Here we show with experiment and simulation that large 3D supercrystals with exceptional order can be assembled by tuning the shape and attraction between polyhedral building blocks. When passivated with adsorbing polymer, Ag nano-polyhedra can behave as quasi-hard particles, and assemble into their densest known packings under a simple gravitational driving force. Excess polymer in solution induces depletion attractions that can stabilize less dense, ordered packings. In the case of octahedra, controlling polymer concentration allows us to tune between the well-known Minkowski lattice, and a novel packing with complex helical motifs. Such large-scale ordered arrangements of Ag nanocrystals provide many possibilities for designing scalable 3D plasmonic metamaterials with applications including chemical and biological sensing, nanophotonics and photocatalysis.

11:51AM J44.00004 Nanoscale systems assembled with DNA: from principles to rational design, OLEG GANG, Brookhaven National Laboratory-Center for Functional Nanomaterials — This abstract not available.

12:27PM J44.00005 A direct comparison of crystallization transitions and glassy dynamics in polymers and colloids¹, ROBERT S. HOY, COREY S. O'HERN, Yale University — Using computer simulations, we compare the freezing transitions in systems composed of N spherical particles with and without covalent-bonding constraints. Linear polymer chains with $N - 1$ permanent covalent bonds are compared to "colloidal" systems with the same nonbonded interactions but no covalent bonds. In the "sticky hard sphere" limit, where covalent bonds act as holonomic constraints, the melting temperatures T_{melt} for both polymers and colloids (with the same N) are inversely proportional to the number of unconstrained degrees of freedom. We also examine the effect of the thermal quench rate $|\dot{T}|$ on collapse. At $|\dot{T}|$ below a lower "critical" value, which decreases rapidly with increasing N , polymers and colloids form similar ground states. This critical value is lower for polymers than colloids and has different N -dependence. In both cases, the dynamics of the systems slow down near T_{melt} as the system approaches isostaticity. For high $|\dot{T}|$, glassy dynamics produces disordered final states. At intermediate $|\dot{T}|$, we find complex nonmonotonic behavior in T , which we relate to the very different rearrangement kinetics of polymeric and colloidal clusters.

¹Support from NSF grant no. CMMT-1006527 is gratefully acknowledged.

12:39PM J44.00006 Dynamics of Fatty Acid Single Molecule Islands on Metal-exchanged Mica, MOURAD CHENNAOUI, ALEKS PONJAVIC, JANET WONG, Imperial College London, London, UK — Under certain conditions, surface-active molecules are known to self-organise into SAMs according to two main driving forces: molecular surface adsorption via diffusive/convective transport, and surface reorganisation and growth. For the latter in-situ methods are required to deconvolute the complex underlying kinetics and dynamics. To this end, a single molecule fluorescence imaging technique is used to observe the dynamics of fatty acid molecules on different metal-exchanged Mica substrates (K, Li, H). It is shown that the molecular surface re-organisation proceeds via an initial islandisation step. These islands spread and grow until forming a stable and organised SAM. Islands formation kinetics/dynamics according to different surface metal types is investigated. Diffusive mechanisms within and between the islands are also explored.

12:51PM J44.00007 Multicompartment and multigeometry nanostructures with block copolymers and kinetic control, DARRIN Pochan, University of Delaware — The combination of charged block copolymer architecture with the kinetic control of solvent processing offers great flexibility for the creation of new assembled morphologies in solution and outstanding ability to control and manipulate those morphologies. When charged, acidic blocks are present, assembled structures are tunable in a well-defined way via co-assembly of organic bases with adjustable chain structure and control of the solution assembly pathway. A rich variety of polymeric micelles have been made such as toroids, disks, and helical cylinders from poly(acrylic acid)-*block*-poly(methyl acrylate)-*block*-polystyrene (PAA-*b*-PMA-*b*-PS) triblock copolymers in THF/water mixtures with multiamines to complex with the PAA. Both the type and amount of multiamine were found to be critical for formation of specific micelles. Kinetic pathways and temporal stabilities of different micelles and nanoscale aggregates have also been studied. Due to low chain exchange dynamics between block copolymeric micelles in solution, global thermodynamic equilibrium is extremely difficult, if not impossible, to achieve. In our block copolymer/THF/water/multiamine quaternary systems, thermodynamics and kinetics of morphological evolution are governed by three important factors, including chain length of hydrophobic blocks, ratio of THF to water, and the interaction of multiamine with hydrophilic PAA block in the corona. Slow kinetics associated with these factors in solution greatly hinders the system from reaching a global equilibrium. However, by taking advantage of slow kinetics behavior of polymeric micelles in solution, one can purposely produce multicompartment micelles and multigeometry micelles by now mixing different PAA-containing block copolymers together but forcing them to ultimately reside in the same nanoscale structure through kinetic processing. While kinetically trapped in common nanostructures, local phase separation can occur producing compartments. This compartmentalization can be used within common micelle geometries to make complex spheres and cylinders or can be used to make new nanostructures such as multigeometry aggregates (e.g. hybrid cylinder-sphere aggregates). All is possible through the kinetic control of the assembly process.

1:27PM J44.00008 Determination of critical micelle concentrations in ionic liquid/block copolymer systems, MICHELLE MOK, TIMOTHY LODGE, University of Minnesota — The micellization of block copolymers in ionic liquids is of great interest, due to their potential as cargo carriers for separations, transfer and extraction applications. In this study, we investigate the critical micelle concentration (cmc) of block copolymers in ionic liquids using fluorescence-based techniques. Specifically, the cmcs of poly(styrene-*b*-ethylene oxide) and poly(styrene-*b*-methacrylate) copolymers were determined from the polarity-sensitive emission spectra of pyrene probes. At the onset of micellization, the probes preferentially partition to the non-polar styrene cores, analogous to pyrene-based cmc studies of aqueous micelle systems. The cmcs are explored as a function of copolymer block molecular weight and composition, as well as ionic liquid composition.

1:39PM J44.00009 Hierarchical Helical-Assembly of Conjugated Poly(3-hexylthiophene)-*b*-poly(3-triethylene glycol-thiophene) Diblock Copolymers, EUNJI LEE, BRENTON HAMMER, TODD EMRICK, RYAN C. HAYWARD, Department of Polymer Science and Engineering, University of Massachusetts, Amherst — One-dimensional crystalline fibrillar assemblies of poly(3-hexylthiophene) (P3HT)-based materials hold significant potential for fabrication of low-cost optoelectronic devices. We have studied the crystallization-driven assembly of a series of poly(3-hexylthiophene)-*block*-poly(3-triethylene glycol-thiophene) (P3HT-*b*-P3TEGT) diblock copolymers, which provide a large contrast in solubility due to the presence of non-polar (hexyl) and polar (TEG) side-chains. P3HT-*b*-P3TEGT diblock copolymers were found to form well-defined fibrillar structures in mixed solvents of chloroform and methanol, with lengths could be tuned easily by changing the solvent composition or relative block lengths. For polymers containing relatively short P3TEGT blocks, the resulting fibers show twisted ribbon-like structures. For appropriate block ratios, complexation of the TEG side chains to alkali metal cations drives formation of clearly defined single helical ribbons and superhelical structures.

1:51PM J44.00010 Molecular simulation study of random block copolymer films prepared through solvent evaporation, DMITRY BEDROV, KEITH HAMBRECHT, GRANT SMITH, University of Utah — Molecular simulations have been used to study equilibrium and non-equilibrium morphologies of random block copolymer films prepared through solvent evaporation. The polymer chains are comprised of “A” and “B” beads connected by FENE springs. Chains comprised of six blocks (ten beads each) and representing all possible combinations of A and B blocks were used to form films with 50/50 A/B fraction. Bead-bead interactions were chosen such that one of the blocks had higher glass transition temperature than the other and that the A and B blocks were incompatible in absence of the solvent. Initially the polymer chains were dissolved in a monomeric solvent at 75/25 solvent/polymer ratio. Then, polymer films were formed through solvent evaporation at various processing parameters. The nanoscale structure and viscoelastic properties of the polymer were investigated as a function of solvent quality, segment incompatibility and rate of evaporation. It was found that when the temperature is below the glass transition temperature of one of homopolymers, the morphology and properties of the film are strongly dependent on evaporation rate.

2:03PM J44.00011 Blood Clotting-Inspired Control of Single-Chain Molecules in Flows, CHARLES SING, ALFREDO ALEXANDER-KATZ, MIT — Recent experimental evidence has demonstrated a clear link between mechanical stimuli and the activation of von Willebrand Factor (vWF), a protein that plays a critical role in the blood clotting cascade. This protein exhibits counter-intuitive conformational and adsorption responses that suggest novel ways of controlling the single-chain dynamics of polymer chains. Specifically, we are using simulation and theoretical approaches to elucidate the fundamental physics that govern globule-stretch transitions in collapsed polymers due to the effect of fluid flows. We begin to extend this general approach to the case of globule adsorption-desorption transitions in the presence of fluid flows, and demonstrate how kinetic considerations must be taken into account to describe the basic features of these transitions. We expect that these results will both allow the development of novel techniques for single-chain targeting and assembly and offer insight into the physiological behavior of vWF.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L9 DFD: Micelles and Vesicles I D220

2:30PM L9.00001 Faceting of multicomponent charged elastic shells, RASTKO SKNEPNEK, CHEUK LEUNG, LIAM C. PALMER, Northwestern University, GRAZIANO VERNIZZI, Siena College, SAMUEL I. STUPP, MICHAEL J. BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University — Combining coarse-grained molecular dynamics simulations with continuum elastic theory, we show that electrostatic interactions between charged lipid head groups can lead to the crystallization of the bilayer. Regions with different molecular charge ratios have distinct elastic properties and naturally tend to segregate inducing an effective line tension between neighboring patches. The line tension and local patch-dependent elastic properties, i.e., bending rigidity and Young modulus, have a drastic effect on the shell shape. We explore a wide region of parameter space and find a gallery of faceted structures, closely resembling shapes of shells recently identified experimentally.

2:42PM L9.00002 Modeling co-evolution of defects and curvature in lipid vesicles: coarse-grained simulation studies¹, ROBIN SELINGER, JUN GENG, JONATHAN SELINGER, Kent State Univ. — To explore interaction between topological defects and curvature in lipid vesicles, we present a coarse-grained simulation approach in which defects and vesicle shape both evolve in time. First we model a vesicle cooled into the tilted gel phase. To represent the tilt field at the mesoscale, we superimpose an XY model onto a coarse-grained liquid membrane [1] where each particle represents a patch of lipid bilayer. The presence of two +1 defects drives the vesicle to a prolate equilibrium state as previously predicted; but extra +1/-1 defect pairs may induce a highly disordered shape which is deeply metastable. We discuss comparison with relevant experiments. Next we consider a lipid vesicle with nematic order, e.g. composed of lipids with a rod-shaped head group. With weak coupling between defects and curvature, the vesicle is spherical with four +1/2 defects. With stronger coupling, the vesicle becomes prolate with two defects clustered at each end. As coupling is further increased, pores nucleate at the defects and coalesce, producing a hollow cylinder. We compare simulation results with theoretical predictions and consider further applications e.g. to study tilt and defects in gel phase lipid rafts.

[1] H. Yuan et al, *Phys Rev E* 82 (2010) 011905

¹Supported by NSF-DMR-0605889.

2:54PM L9.00003 Coarse-grained model for lipid bilayer membranes and vesicles¹, JUN GENG, JONATHAN SELINGER, ROBIN SELINGER, Kent State Univ. — We present a coarse-grained model for simulation studies of lipid bilayer membranes and vesicles. We separately track the behavior of the leaflets in each bilayer, allowing us to model the mechanics of vesicles and a rich array of other phases, topologies, and defect structures. Each particle in the coarse-grain model represents a patch of lipid molecules and carries a vector degree of freedom, representing the local average lipid chain orientation. Particles interact via a pair potential depending on separation distance and relative chain orientation. Solvent is treated as implicit, and membrane fluctuations are modeled via a Langevin thermostat. Resulting bilayer structures show liquid-like diffusion within each leaflet. We show that bilayer vesicles coalesce spontaneously from a random initial state, even though no spontaneous curvature is imposed by the model. We also explore the transition from vesicles to lamellar phases as a function of increasing density. We discuss potential application to the study of vesicle fission and fusion.

¹Work supported by NSF-DMR-0605889

3:06PM L9.00004 Molecular dynamics study of shape transitions in aqueous micelle solutions¹

, A. SANGWAI, R. SURESHKUMAR, Syracuse University, Syracuse, NY 13244, USA. — It is well known that surfactant molecules self-assemble in aqueous solutions to form various micellar structures such as spheres, rods or sheets. Although this phenomenon is widely studied experimentally, the molecular mechanisms of shape transitions are not well understood. Atomistic simulations of self-assembled micellar systems are computationally prohibitive to sample several hundred nanoseconds necessary to capture shape transitions. We demonstrate that MARTINI coarse-grained (CG) force field for CTAC is capable of accurately representing micellar assemblies by comparing the CG system to fully atomistic ones. Microsecond molecular dynamic simulations using MARTINI CG models in explicit water are used to predict sphere to rod transitions in micelles. Inter-micelle association free energies are estimated to distinguish between the chemical environments in which the micelle assumes a spherical versus rod-like shape. Presence of hydrophobic salt e.g. Sodium Salicylate, is shown to greatly promote the formation of rodlike structures. CG MARTINI molecular dynamics is benchmarked as a practical approach to study nano-scale micellar structures.

¹NSF Grant 1049454

3:18PM L9.00005 Ordered bulk aggregates of lipid vesicles, ANA HOCEVAR, Jozef Stefan Institute, PRIMOZ

ZIHERL, Faculty of Mathematics and Physics, University of Ljubljana and Jozef Stefan Institute — We study the structure of bulk assemblies of identical lipid vesicles. In our model, each vesicle is represented as a convex polyhedron with flat faces, rounded edges, and rounded vertices. Each vesicle carries an elastic and an adhesion energy and it turns out that in the limit of strong adhesion, the minimal-energy shape of cells minimizes the weighted total edge length. We calculate the shape of the rounded edge exactly and show that it can be well described by a cylindrical surface. We compare several candidate space-filling polyhedra and we find that the oblate shapes are preferred over prolate shapes for all volume-to-surface ratios. We also study aggregates of vesicles whose adhesion strength on lateral faces is different from that on basal/apical faces. We determine the anisotropy needed to stabilize prolate shapes and we show that at any volume-to-surface ratio, the transition between the oblate and the prolate shapes is very sharp. We compare the geometry of the model vesicle aggregates with the shapes of cells in certain simple animal tissues. Predictions of our model are consistent with available experimental data.

3:30PM L9.00006 Understanding crumpling lipid vesicles at the gel phase transition¹, LINDA

HIRST, School of Natural Sciences, University of California, Merced, ADAM OSSOWSKI, MATTHEW FRASER, University of California, Merced — Wrinkling and crumpling transitions in different membrane types have been studied extensively in recent years both theoretically and computationally. There has also been very interesting recent work on defects in liquid crystalline shells. Lipid bilayer vesicles, widely used in biophysical research can be considered as a single layer smectic shell in the liquid crystalline phase. On cooling the lipid vesicle a transition to the gel phase may take place in which the lipid chains tilt and assume a more ordered packing arrangement. We observe large scale morphological changes in vesicles close to this transition point using fluorescence microscopy and investigate the possible mechanisms for this transition. Confocal microscopy is used to map 3D vesicle shape and crumpling length-scales. We also employ the molecular tilt sensitive dye, Laurdan to investigate the role of tilt domain formation on macroscopic structure.

¹Funded by NSF CAREER award (DMR - BMAT #0852791).

3:42PM L9.00007 Thin shell vesicles composed of hydrophilic plate-like nanoparticles, ANAND

SUBRAMANIAM, School of Engineering and Applied Sciences, Harvard University, JIANDI WAN, Department of Mechanical and Aerospace Engineering, Princeton University, ARVIND GOPINATH, Fischer School of Physics, Brandeis University, HOWARD STONE, Department of Mechanical and Aerospace Engineering, Princeton University — Nanopowders of graphene oxide, montmorillonite and laponite spontaneously delaminate into ultrathin nanoscopic plates when dispersed in water. These plates, which are typically ~ 1 nm thick and microns in lateral dimension, have found many uses as precursors to graphene, ceramics, layer-by-layer structures, and as structural modifiers of nanocomposites. Here we show that mechanical forces due to shear in a narrow gap can assemble hydrophilic plate-like particles on air bubbles, forming stable nanoplated armored bubbles. Translucent inorganic vesicles (vesicles defined here as closed thin-shelled structures with the same liquid inside and outside) of these particles are produced when the nanoplated armored bubbles are exposed to common water-miscible organic liquids and surfactants. These inorganic vesicles are mechanically robust, have walls that are about six nanometres thick, and are perforated with pores of submicron dimensions. We characterize the phenomenon and find that a wetting transition at the scale of the nanoparticles is the primary mechanism of formation. The discovery of these novel inorganic structures raises a wealth of questions of fundamental interest in materials and surface science.

3:54PM L9.00008 The effect of interlayer distance of thickness fluctuations in a swollen lamellar phase: A neutron spin echo study, MICHIIHIRO NAGAO, NIST Center for Neutron Research and Indiana University —

Thickness fluctuations in surfactant membranes have been measured using small-angle neutron scattering (SANS) and neutron spin echo (NSE) techniques as a function of the membrane thickness in a swollen lamellar structure composed of nonionic surfactant, water and oil. An excess dynamics from the bending motion was observed around the length scales of the membrane thickness, which originates from thickness fluctuations of the membranes. The amount of oil in the bilayers controls the interlayer distance (membrane thickness) and the bending motion of the membranes. An enhancement of the thickness fluctuations suppresses the bending motion, which introduces the increase in the bending modulus at low swelling condition. The decrease in the bending modulus with further increase in the thickness indicates the decrease of the synchronization between monolayers. In the high swelling conditions, the monolayer movement dominates the dynamics of the membranes in the measured dynamic range.

4:06PM L9.00009 The effect of interlayer distance on thickness fluctuations in a swollen lamellar phase: A molecular dynamics study, SUKHUM CHAWANG, The University of Oklahoma, TAKUMI HAWA, The University of Oklahoma —

Molecular dynamics simulations have been conducted to characterize thickness fluctuations in a swollen lamellar structure, composed of a non-ionic surfactant, water, and oil, to verify the results of the neutron scattering experiments by Nagao. The thickness fluctuations are measured as an excess dynamics from the bending motion around the length scales of the membrane thickness and as a function of the interlayer distance (membrane thickness). The enhancement of the thickness fluctuations is observed in all ranges of thickness we simulated; however, it decays with increase of the membrane thickness. Dependence of directions of sampling wave vectors q on the thickness fluctuation is also investigated. At more normal direction (perpendicular to the membrane surfaces) the excess dynamics is clearly observed, while at more lateral direction (parallel to the membranes) the bending motion is more clearly observed. The present results show the existence of the enhancement of the thickness fluctuations and the importance of the sampling directions.

4:18PM L9.00010 Studies of lipid vesicle mechanics using an optical fiber dual-beam trap¹,

TESSA M. PINON, School of Engineering-University of California, Merced, LINDA S. HIRST, JAY E. SHARPING, School of Natural Sciences-University of California, Merced — Fiber-based optical traps can be used for manipulating micron-sized dielectric particles such as microspheres and biological cells. Here we study the mechanics of giant unilamellar vesicles (GUVs) which are held and stretched by light forces in a fiber-based dual-beam optical trap. Our GUVs are suspended in a buffer solution and encapsulate various concentrations and molecular weights of poly(ethylene glycol) (PEG) polymer yielding a range of refractive index contrasts and trapping conditions. We find that we can trap GUVs in solution with index contrasts of less than 0.01. We explore the mechanical response of the GUV membrane to a range of forces which are proportional to laser power and refractive index contrast. Our trapping system is a compact and inexpensive platform and trapping is viewed in real time under a microscope. We hypothesize that forces within the high-tension regime will induce a linear response in vesicle surface area. This project sets the stage for membrane mechanics and lipid phase change studies.

¹Grant: NSF award #DMR 0852791, "CAREER: Self-Assembly of Polyunsaturated Lipids and Cholesterol in the Cell Membrane"

4:30PM L9.00011 Thermal Stress of Supported Lipid Bilayer Induces Formation and Collapse of Uniform Radius Tubules, KIMBERLY WEIRICH, DEBORAH FYGENSON, University of California, Santa Barbara — Supported lipid bilayer (SLB) provides a model system in which to quantitatively investigate fluid bilayer transitions from planar to tubular and tubular to spherical morphologies. Following a small increase in temperature, flexible filaments extrude from a fluid SLB. Individual filaments can reach hundreds of microns in length before spontaneously collapsing into discs. We demonstrate that the filaments are tubular and report the effects of lipid composition and flow-induced tension on their properties. At high ionic strength, the sub-resolution tubules are adsorbed to the SLB, enabling the measurement of their radius to within ± 5 nm using fluorescence microscopy.

4:42PM L9.00012 A Time-Resolved Study on Nanodisc-to-Vesicle Transformation, MU-PING NIEH, IMS/CMBE, University of Connecticut, SUANNE MAHABIR, WAN KEI WAN, University of Western Ontario, JOHN KASTARAS, Oak Ridge National Lab/CNBC — Structural phase diagram of a phospholipid mixture composed of dimyristoyl phosphatidylcholine (DMPC), dihexanoyl phosphatidylcholine (DHPC) and dimyristoyl phosphatidylglycerol (DMPG) contains many rich morphologies, e.g., nanodiscs also known as "bicelles", bilayered ribbons, unilamellar vesicles (ULVs), multi-lamellar vesicles (MLVs) and perforated lamellae. In this report, we will present time-resolved small angle neutron scattering and dynamic light scattering measurements of the structural transformation from nanodiscs to ULVs as a function of temperature, lipid concentration and charge density. The result will reveal the growth rate of nanodiscs and all the intermediate structures along the transformation process. Through the understanding of the kinetic pathway, the size and polydispersity of the self-assembled nano-size ULVs can be well-controlled. These ULVs can be used as a carrier for therapeutics or imaging probes.

4:54PM L9.00013 Crystallization Induced by Electrostatic Correlations in Vesicles of Mixed-Valence Ionic Amphiphiles¹, CHEUK YUI LEUNG, RASTKO SKNEPNEK, LIAM PALMER, GRAZIANO VERNIZZI, MEGAN GREENFIELD, SAMUEL STUPP, MICHAEL BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University — Charged amphiphilic molecules, including molecules with biological motifs, have been predicted to organize into elastic membrane or crystalline shells with non-spherical shapes. We demonstrate that pure electrostatic interaction allow (-1) anionic water insoluble amphiphiles and (+3) cationic amphiphiles, which form only micelles in water, to co-assemble into buckled vesicles. The strong interaction between the +3 and -1 head groups increases the cohesive energy of the amphiphiles and favors the formation of crystallized membranes or shells that facet spontaneously into buckled shapes predicted by simulations of vesicles with heterogeneous elastic properties. In situ small-angle and wide-angle X-ray scattering (SAXS-WAXS) experiments conducted at the Advanced Photon Source DND-CAT confirm the presence of crystalline bilayers. Our simulations verify that ionic lateral correlations among the oppositely charged head groups of the co-assembled amphiphiles are responsible for the observed tail crystallization.

¹This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering (DOE Contract No. DE-FG02-08ER46539)

5:06PM L9.00014 Endocytic internalization of nanoparticles into polymeric vesicles., ANJA KROEGER, KARMENA JASKIEWICZ, Max Planck Institute for Polymer Research, ANTJE LARSEN, Department of Materials Science and Technology, University of Crete and F.O.R.T.H., GEORGE FYTAS, Department of Materials Science and Technology, University of Crete and F.O.R.T.H. and Max Planck Institute for Polymer Research — The monitoring of transport through cell membranes is essential for proper functioning of all living organisms. Poorly understood mechanisms of endocytosis have become the focus of intense investigations. Here we present a photon correlation spectroscopy study of the uptake of polystyrene nanoparticles (hydrodynamic radius, $R_h=16$ nm) by poly(dimethylsiloxane)-b-poly(2-methyloxazoline) polymersomes ($R_h=150$ nm) in aqueous solution. The relaxation function $C(q,t)$ for a particle/polymersome mixture with a molar ratio 100:1 at different scattering wave vectors (q) reveal the presence of free and bound particles. Both the experimental form factor $P(q)$ and the effective diffusion coefficient $D(q)$ of the polymersome in the q -range of 0.005 - 0.033 nm⁻¹ are consistently described by modeling these q -patterns by a filled polymersome with about 30 particles under the examined conditions. The emerged picture is supported by cryo-TEM imaging.

5:18PM L9.00015 AC-Electrokinetic Characterization and Induced Encapsulation Release of Micelles in Aqueous Suspensions, VICTORIA FROUDE, YINGXI ELAINE ZHU, University of Notre Dame — Micelles and polymers vesicles have been of increasing interest as drug delivery systems for controlled release, specific cell targeting, and medical diagnostics. In addition, AC-electrokinetic techniques have emerged as a viable option for colloidal and biocolloidal manipulation. In this work, we examine the dielectrophoresis (DEP) characteristics of complex micellar nanoparticles under non-uniform AC-electric field of varied ac-field frequencies (5 kHz-20 MHz) and amplitudes (0.1-10 Vpp) by fluorescence correlation spectroscopy (FCS) at a single-molecule resolution. We focus on the AC-field induced transport of sodium tetradecyl sulfate (STS) and sodium dodecyl sulfate (SDS) micelles tagged with various fluorescent and drug encapsulates in aqueous media. We observe a strong AC-frequency dependence of micelle concentration between two microelectrodes, from which the DEP crossover frequency is determined. Surprisingly, we also observe an AC-field induced dissociation of the micelle structure and a resulting release of fluorescent encapsulates at a characteristic low AC-field frequency of approximately 1-10 kHz, where the dissociation has been found to be dependent on the surface charge of the interior encapsulate.

Wednesday, March 23, 2011 8:00AM - 11:00AM –
Session P9 DFD: Liquid Crystals: Smectics, Nano-mixtures D220

8:00AM P9.00001 Achiral structure of B4 phase in a Bent-Core Liquid Crystal¹, DONG CHEN, MICHAEL-SCOTT HEBERLING, JOSEPH MACLENNAN, MATTHEW GLASER, NOEL CLARK, Liquid Crystal Materials Research Center, University of Colorado at Boulder, HIDEO TAKEZOE, Department of Organic and Polymeric Materials, Tokyo Institute of Technology — Bent-core smectic layers have a tendency to exhibit spontaneous saddle-splay curvature, driven by the intra-layer structural mismatch. In the chiral B4 phase, the tendency for twist in the orientation of neighboring molecules coupled with the saddle-splay curvature lead to the formation of helical nanofilaments with either clockwise or anticlockwise twist. In addition to the helical nanofilament structure, we observe another microscopic structure in P12OP1MB, which is achiral, with no helical twist. This coffee-bean-like microstructure is dominated by saddle-splay curvature, like the dark conglomerate phase, but appears to have three dimensional order. The origin of these structures will be discussed.

¹This work is supported by NSF MRSEC Grant DMR0820579 and NSF Grant DMR0606528.

8:12AM P9.00002 Two ferroelectric phases in a bent-core liquid crystal , C. ZHANG, N. DIORIO, B.K.

SADASHIVA, A. JÁKLI — We report electro-optical, polarization current, dielectric and SAXS studies on novel bent-core materials that contain four ester groups; three in one arm and only one in the other. These materials differ from each other only by the number of carbons (n) in the alkoxy chain terminating the one ester containing arm: in Ar 35 $n=14$, while in Ar 39 $n=18$. The phase sequences of Ar 35 and 39 are very similar to each other. Both have two mesophases, M1 and M2, with M1 in the 115°C-140°C temperature range, and M2 in between about 100°C and 115°C. Polarization current measurements indicate polarization current and optical switching in the M₁ phase with spontaneous polarization and switching time in the P_s~2.5-3mC/m² and $\tau \sim 200\mu$ s range, respectively. While in Ar 35 the M2 phase cannot be switched, in the AR 39 we could detect polarization switching with a polarization value of about 5-6 mC/m² and switching time over a millisecond. Dielectric and X-ray scattering studies were employed to reveal the fine structure of the M₁ and M₂ phases.

8:24AM P9.00003 Surface Induced Reduction of Twisting Power in Liquid Crystal Films ,

LIDONG PAN, University of Minnesota, CHENG-CHER HUANG — Null transmission ellipsometry was employed to study the temperature evolution of the helical structure in smectic liquid crystal films. Free standing films with thickness ranging from 31 to more than 400 layers were prepared and studied. The experimental results show a reduced twisting power in thin films. A simple model was constructed to explain the results. Surface effect was found to be the reason for this phenomenon. Our findings are consistent with the studies of helically ordered magnetic films.

8:36AM P9.00004 Evolution of the isotropic to smectic-A phase transition in liquid crystal and acetone binary mixtures , KRISHNA SIGDEL, GERMANO IANNACCHIONE, Worcester Polytechnic Institute —

The first-order transition from the isotropic (I) to smectic- A (SmA) phase in the liquid crystal 4-cyano-4'-decylbiphenyl (10CB) doped with the polar solvent acetone (ace) has been studied as a function of solvent concentration by high-resolution ac-calorimetry. Heating and cooling scans were performed for miscible 10CB+ace samples having acetone mole fractions from $x_{ace} = 0.05$ (1 wt.%) to 0.36 (10%) over a wide temperature range from 310 to 327K. Two distinct first-order phase transition features are observed in the mixture whereas there is only one transition (I - SmA) in the pure 10CB for that particular temperature range. Both calorimetric features reproduce on repeated heating and cooling scans and evolve with increasing x_{ace} with the high temperature feature relatively stable in temperature but reduced in size while the low temperature feature shifts dramatically to lower temperature and exhibits increased dispersion. Polarizing optical microscopy supports the identification of a smectic phase below the high-temperature heat capacity signature indicating that the low-temperature feature represents an injected smectic-smectic phase transition. These effects may be the consequence of screening the intermolecular potential of the liquid crystals by the solvent that stabilizes a weak smectic phase intermediate of the isotropic and pure smectic- A .

8:48AM P9.00005 The Power of Poincaré: Elucidating the Hidden Symmetries in Focal Conic

Domains , ELISABETTA A. MATSUMOTO, GARETH P. ALEXANDER, BRYAN GIN-GE CHEN, RANDALL D. KAMIEN, Department of Physics and Astronomy, University of Pennsylvania — Focal conic domains are typically the “smoking gun” by which smectic liquid crystalline phases are identified. The geometry of the equally spaced smectic layers is highly generic but, at the same time, difficult to work with. We develop an approach to the study of focal sets in smectics which exploits a hidden Poincaré symmetry revealed only by viewing the smectic layers as projections from one-higher dimension. We use this perspective to shed light upon the concentric cyclides of Dupin and several classic focal conic textures which exhibit a more widespread level of geometric organization as in Friedel's law of corresponding cones, the networks and trellises expounded by Bouligand, or Apollonian packings.

9:00AM P9.00006 Phase behavior of platelets at different aspect ratios , ANDRES MEJIA, YA-WEN CHANG,

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77843, DAZHI SUN, Department of Mechanical Engineering, Texas A&M University, College Station, TX 77843, AGUSTIN DIAZ, ABRAHAM CLEARFIELD, Department of Chemistry, Texas A&M University, College Station, TX 77843, HUNG-JUE SUN, Department of Mechanical Engineering, Texas A&M University, College Station, TX 77843, ZHENG DONG CHENG, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77843 — Suspensions of α -ZrP monolayer plates have recently been found to exhibit an isotropic to nematic (I-N) and nematic to smectic (N-S) phase transition. In the past, computer simulations have been developed to study the phase diagrams of platelets. In order to experimentally investigate the phase transitions and rheological behaviors of these particles, it is necessary to be able to manipulate their size, thickness and reduce their size distribution. We demonstrate here the strong dependency of the I-N transition on the aspect ratio (diameter/thickness) via the control of pristine α -ZrP platelets. We confirmed that the I-N transition volume fraction decrease monotonically with the aspect ratio as shown in previous simulations by J.A.C. Veerman and D. Frenkel. Furthermore, we found additional isotropic and gel phases by increasing the polydispersity of platelet sizes.

9:12AM P9.00007 Liquid Crystal-ZnO Nanoparticle Potential Photovoltaics: Role of LC Order and ZnO Particle Size and Concentration¹ , LUZ J. MARTINEZ-MIRANDA, JANELLE BRANCH², ROBERT THOMPSON,

JEFFERSON W. TAYLOR, LOURDES SALAMANCA-RIBA, University of Maryland — We investigate the role order plays in the transfer of charges in ZnO nanoparticle - 8CB liquid crystal system for photovoltaic applications as well as the role the nominally 5x7nm² ZnO nanoparticles play in improving that order. Our results for the 5nm nanoparticles show an improvement in the alignment of the liquid crystal with increasing weight percentage of ZnO nanoparticles, up to a concentration of 30% wt for the 5nm particles accompanied by an increase by three orders of magnitude in the current generated.³ Our results for the 5 x 7 nm² sample show that the current is larger than the current obtained for the 5 nm samples. The photocurrent can be expressed as the conductivity as a function dependent in the order in the sample times the portion of the electric field that is absorbed and transformed into the current.

¹This work was supported by NSF-DMR- MRSEC-0520471, and its REU program, and in part by NSF-DMR-0906433.

²UMCP REU participant from Florida Institute of Technology

³L. J. Martínez-Miranda, Kaitlin M. Traister, Iriselies Meléndez-Rodríguez, and Lourdes Salamanca-Riba, Appl. Phys. Letts, 97, in press (2010).

9:24AM P9.00008 Interaction of a Bi-molecular Liquid Crystal Film With Functionalized Nanoparticles¹ , JEFFERSON W. TAYLOR, LUZ J. MARTINEZ-MIRANDA, University of Maryland, LYNN K. KURIHARA, Naval Research Labs

— We investigate the properties of a nominally bi-molecular film of liquid crystal mixed with a magnetic nanoparticle (CoFe) that was functionalized with an organic compound (MHDA or APTS) with the atomic force microscope (AFM). We seek to investigate if the functionalization compound has an effect on the ordering of the liquid crystal in the vicinity of the nanoparticle. Studies in bulk liquid crystals have shown that the functionalization compound influences how the liquid crystal will reorganize.² The results of this investigation are compared to the results of work done on phospholipids in close contact with uncovered silica nanoparticles.³ There seems to be a relation between the way that the two functionalizations behave in the bulk 8CB. The two functionalizations studied behave differently for particles larger than 22 nm, and apparently for the smaller particles.

¹This work was supported by NSF-DMR-0906344.

²L. J. Martínez-Miranda, and Lynn Kurihara, *J. Appl. Phys*, *105*, p. 084305 (2009).

³Yuri Roiter, Maryna Ornatska, Aravind R. Rammohan, Jitendra Balakrishnan, David R. Heine, and Sergiy Minko, *Langmuir*, *25*, 6287-6299 (2009).

9:36AM P9.00009 Directed assembly of CdSe/ZnS quantum dots in cholesteric liquid crystal matrix, ANDREA RODARTE, LINDA S. HIRST, SAYANTANI GHOSH, University of California, Merced — Controlled self assembly of quantum dots (QDs) over macroscopic scales is important to realizing the potential for new applications such as photovoltaic devices and sensors. Here, we suspend CdSe/ZnS core/shell QDs in a cholesteric liquid crystal (LC) and investigate the dispersion and collective emission of the QDs when loaded into a Grandjean-Cano wedge cell. We use polarized optical microscopy and scanning photoluminescence microscopy to generate spatial and spectral maps of the QD-liquid crystal samples. We find that the LC forms Grandjean steps approximately 200um in width and the spectral effects of the QD emission correlate to the stripe formation. We also find that the cholesteric LC modulates the spectral emission of the QDs, creating a wavelength gradient dependant on the orientation of the collection polarizer with the director axis of the liquid crystal molecules.

9:48AM P9.00010 ABSTRACT WITHDRAWN —

10:00AM P9.00011 Diffusion-controlled Aggregation of Bucky Balls on Freely Suspended Smectic Liquid Crystal Films, ZOOM NGUYEN, TATYANA MALININA, CHEOL PARK, JOSEPH MACLENNAN, MATTHEW GLASER, NOEL CLARK, University of Colorado-Boulder, LIQUID CRYSTAL MATERIALS RESEARCH CENTER TEAM — Bucky balls (BB) have the tendency to clump together, making it hard to have them suspended in a solvent. We find that in highly viscous bulk 8CB, a smectic liquid crystal at room temperature, the aggregation happens more slowly. As the result, a freely suspended film made from the 8CB-BB mixture contains mostly small BB clumps. The diffusion coefficients of the clumps in thin films are much bigger than in the bulk, however, accelerating the aggregation process. We measure, via video microscopy, the decrease of the clumps' diffusion coefficients over time, indicating that their sizes increase towards a terminal size determined from the rate of diffusion. The terminal-sized clumps still diffuse around and stick to each other when they meet, forming the classic fractal pattern.

10:12AM P9.00012 Investigation of the lyotropic liquid crystal phase of Graphene Oxide solution¹, YUE SHI, RIZWAN MAHMOOD, DONG CHEN, NOEL CLARK — Graphite Oxide spontaneously exfoliates into single-layer Graphene Oxide flakes in water. As the concentration becomes higher, Graphene Oxide solution shows a phase transition from the isotropic to the lyotropic liquid crystal phase. In the liquid crystal phase, the Graphene Oxide flakes can be ordered spontaneously by flow and shearing forces. We will report the investigation of the liquid crystal phase of the Graphene Oxide solution. In addition, the light scattering studies give dynamic information of the Graphene Oxide solution. Both the translational and rotational diffusion properties are investigated corresponding to different phases formed by Graphene Oxide at different concentrations.

¹Supported by NSF MRSEC Grant DMR0820579.

10:24AM P9.00013 Defect dynamics in monodomain formation of a lyotropic chromonic liquid crystal under confinement, XUXIA YAO, Georgia Tech, ALEJANDRO REY, McGill University, JUNG PARK, MOHAN SRINIVASARAO, Georgia Tech — Lyotropic chromonic liquid crystals are a relatively new class of liquid crystals. We have studied the process of monodomain formation and the associated defect dynamics of an anionic dye, Sunset Yellow FCF(SSY), under confinement in a flat capillary. SSY solutions were filled into a flat capillary by capillary action in isotropic phase and subsequently cooled to nematic state. Defect coarsening processes due to confinement include growth of small uniform domains, splitting of a center disclination line (+1) into two lines (+1/2), merging of uniform domains, and relaxation of defect curvature after pinch-off. Previously we studied the kinematics of a branch point involving a +1 and two +1/2 intersecting lines. Here we report on the collision of two such branch points and the subsequent emergence of two curved +1/2 lines that eventually coarsen into two parallel lines close to the edge of the capillary. A model that includes bending and tension line elasticity describes the branch point post collision and provides the means to assess viscoelastic moduli.

10:36AM P9.00014 Thermotropic Gold Nanorod Liquid Crystal Phases¹, PAUL LUCHETTE, PETER PALFFY-MUHORAY, Liquid Crystal Institute - KSU — Large scale, oriented arrays of gold nanorods (Au NR) are of interest for a variety of applications, such as negative index materials and hyperbolic dispersion lenses. We report a method for preparing lyotropic, nematic LC phases of Au NR by combining polymer coated Au NR with a low molecular weight (< 3200) polymers solvent. The solvent system was prepared by reacting hydroxymethyl siloxane and styrene via a hydrosilylation reaction. At appropriate ratios, these mixtures exhibit liquid crystalline phase behavior. Lyotropic LC phases of Au NR were observed for Au NR with aspect ratio above 4, diameter ~15nm, using either linear or cyclic siloxane-styrene polymers as the solvent. Compared with other preparation methods such as lithography or evaporative deposition that produce static films, these self-assembled thermotropic LC phases of Au NR may be re-oriented in response to thermal or electric stimulus.

¹This work was supported by the AFOSR under MURI grant FA9550-06-1-0337

10:48AM P9.00015 Organic-Inorganic Liquid Crystalline Composites, PETR SHIBAEV, Department of Physics, Fordham University, New York — Design of novel liquid crystalline composites consisting of organic liquid crystals, metal oxides (titanium oxide, zinc oxide, etc.) and "interface" layer covering inorganic materials is presented and discussed. The composites respond to light irradiation by changing orientation of liquid crystalline molecules, resulting in the changes of transmission and reflection properties of cells made of composite materials. The interaction of composite materials with light results from a complex chain of physico-chemical processes inside both the inorganic component and the "interface" layer. The processes that play the major role in the re-orientation of liquid crystalline molecules in the surface layer include: i. light-induced formation of electron-donor pairs inside metal oxides, ii. energy transfer of electron excitations to molecules inside the "interface" layer, iii. breaking of hydrogen bonds and conformational changes of molecules inside the "interface" layer. The experimental study of the processes resulting in re-orientation of liquid crystals by light is accompanied by theoretical calculations of conformational changes inside the "interface" layer and molecular re-orientation on the surface of inorganic materials.

Wednesday, March 23, 2011 11:15AM - 2:03PM —
Session Q9 DFD: Fluid Dynamics at Interfaces D220

11:15AM Q9.00001 Slosh dynamics and rebound suppression of a partially filled sphere, TAYLOR KILLIAN, Brigham Young University Dept. Mathematics, ROBERT KLAUS, TADD TRUSCOTT, Brigham Young University Dept. Mechanical Engineering — We introduce a study on the slosh dynamics of a partially filled elastic sphere. Currently the physical design of fluid-filled containers utilizes clever construction and machinery to mitigate sloshing motions. There are numerous cases that have been observed but we focus on the impact of a sphere under free fall with an initially undisturbed free surface. The study focuses on measurement and simulation of the force distribution between the fluid and the sphere through the use of high-speed imaging and finite element analysis. Using the cavity shape data, a potential flow numerical model is developed that predicts the unsteady forces. Our hypothesis is that the sphere's movements can be counteracted or cancelled by the exchange of energy between the sphere and the fluid. Forces are modulated by the formation of a parabolic cavity in the fluid, formed after the first impact. The second impact results in a collapse of this cavity forming a powerful jet which effectively dampens the motion of the sphere.

11:27AM Q9.00002 Shrinking Instabilities of Toroidal Liquid Droplets in The Stokes Flow Regime, ZHENWEI YAO, MARK BOWICK, Syracuse University — We analyze the stability and dynamics of toroidal liquid droplets. In addition to the Rayleigh instabilities akin to those of a cylindrical droplet there is a shrinking instability that is unique to the topology of the torus and dominates in the limit that the aspect ratio is near one (fat tori). We first find an analytic expression for the pressure distribution inside the droplet. We then determine the velocity field in the bulk fluid, in the Stokes flow regime, by solving the biharmonic equation for the stream function. The flow pattern in the external fluid is analyzed qualitatively by exploiting symmetries. This elucidates the detailed nature of the shrinking mode and the swelling of the cross-section following from incompressibility. Finally the shrinking rate of fat toroidal droplets is derived by energy conservation.

11:39AM Q9.00003 Normal elasticity of liquid bridge by atomic force microscope¹, BONGSU KIM, WONHO JHE, Seoul National University, CENTER FOR NANO-LIQUID TEAM — The quartz tuning-fork based atomic force microscope (QTF-AFM) has previously been established as a suitable measurement technique for investigating liquid bridges. By operating a QTF-AFM in the non-contact tapping mode, we are able to measure the normal elasticity of liquid bridges that are formed via capillary condensation or that result from an adsorbed liquid layer. Elasticity, a property typically associated with solids, is studied here for the case of the nano-scale water bridge. We present results that add to our understanding of the origin of the elasticity in nano liquid bridges.

¹Work supported by Korean Ministry of Science and Technology.

11:51AM Q9.00004 Droplet impact and the dynamics of rapidly moving contact lines, SHMUEL M. RUBINSTEIN, JOHN M. KOLINSKI, Harvard University, SHREYAS MANDRE, Brown University, LAKSHMINARAYANAN MAHADEVAN, DAVID A. WEITZ, Harvard University — When a liquid drop approaches a flat solid surface, the air beneath it is compressed, flattening the bottom of the drop and forcing initial contact to occur in a ring-shape, trapping a pocket of air in its center as two wetting fronts rapidly expand both outward and inwards to completely wet the surface. We combine total internal reflection (TIR) microscopy with a novel virtual frame technique (VFT) to directly observe the sub-micron length scales above a solid surface as the drop approaches, impacts and then spreads over it.

12:03PM Q9.00005 Interfacial Effects on Droplet Dynamics in Poiseuille Flow, JONATHAN SCHWALBE, KENDRA ERK, National Institute of Standards and Technology, JEFFREY MARTIN, Unilever, PETIA VLAHOVSKA, Brown University, STEVEN HUDSON, National Institute of Standards and Technology — Interfacial rheology governs many properties of emulsions, and here we report theory and experiments that account for and measure surface viscous and elastic forces. For the theoretical portion, Stokes flow is assumed in bulk phases and a jump in hydrodynamic stress at the interface is balanced by Marangoni and surface viscous forces according to the Boussinesq-Scriven constitutive law. Our model employs linear equation of state for the surfactant. Our analysis predicts slip, cross-stream migration and droplet-circulation velocities for a spherical drop in plane Poiseuille flow. These results and the corresponding interfacial parameters are separable: e.g., cross-stream migration occurs only if surfactant is present; slip velocity depends on viscosity contrast and dilatational Boussinesq number, but not shear Boussinesq number. Drop dynamics in plan Poiseuille flow are measured experimentally using microfluidics, particle velocimetry, and shape analysis. Several types of surfactant-stabilized aqueous drops in oil are examined and the interfacial properties depend on interfacial composition.

12:15PM Q9.00006 ABSTRACT WITHDRAWN —

12:27PM Q9.00007 Nonequilibrium molecular dynamics of vapor–liquid interface, TAKERU YANO, Osaka University, Japan — Evaporation and condensation at a vapor–liquid interface are studied by moderately large-scale nonequilibrium molecular dynamics simulations for a vapor–liquid two phase system composed of about 0.3 million Lennard-Jones molecules. Constant evaporation and condensation are realized by driving two vapor regions on the either side of a planar liquid film, and thereby the simulation is free from artificial controls of molecular motions in the liquid film and in the neighborhood of the interfaces. This enables us to evaluate the mass, momentum, and energy fluxes across the system, which are relevant to the velocity distribution of molecules leaving the interface at the vapor–liquid nonequilibrium states.

12:39PM Q9.00008 Evaporation out of a 2D model soil, BERTRAND SELVA, REMI DREYFUS, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn UMI 3254, Bristol, Pennsylvania 19007, USA — Our goal is to improve our understanding of water transport in the soil-plant-atmosphere continuum. For this purpose, we focus on water losses due to evaporation at the soil surface. Such losses are known to be important at places where plants do not entirely cover the surface. Our model soil is a 2D porous medium with controlled wettability and humidity. It has been reported that evaporation is characterized by three stages: a first stage with a strong and constant evaporation flux, a second stage where mass transfer is dominated by diffusion mechanisms, and a third stage that occurs when the medium is almost empty. Here we focus on the first two stages and the transition between them which occurs when an intermediate unsaturated zone has reached its maximum width. This width strongly depends on the wettability distribution of the porous medium. In our experiments, we have explored a regime where gravity effects and capillary forces have similar contributions. In this particular regime we found that the first stage is characterized by a continuously decreasing evaporation flux and the second stage by usual diffusion transfer mechanisms. In order to understand this behavior, we have developed a model which allows us to predict the transition between the two stages and which is in agreement with the decreasing values of the first stage evaporation flux.

12:51PM Q9.00009 Effects of Sub-Phase Thickness on Interfacial Microrheology, PAUL CHRISTOPHEL MARTIN, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — The interface between two fluids is known to have a rheological response. In our work, we study human serum albumin protein molecules (HSA) at an air-water interface. Prior experimental work showed that the ratio of the surface viscosity to the sub-phase “bulk” viscosity influences the rheology of the HSA interface. Recent theoretical work has shown that the thickness of the sub-phase h can also influence the rheology of the interface. The finite thickness of the sub-phase only becomes important once h is on the order of the ratio of the surface viscosity to the sub-phase “bulk” viscosity, which is on the order of 100 microns for an HSA-air-water interface. To characterize the interfacial rheology, we suspend tracer particles at the interface, measure their correlated motions, and investigate how the results depend on h for water layers $O(100)$ microns thick.

1:03PM Q9.00010 Probing single- and multi-phase flow at the pore level, SUJIT DATTA, Department of Physics, Harvard University, AMBER KRUMMEL, Department of Chemistry, Colorado State University, DAVID WEITZ, Department of Physics, Harvard University — We use a new experimental technique to study 3D flow behavior in a porous medium in situ with high spatiotemporal resolution. At the multi-pore level, we probe the fluid configurations resulting from two-phase flow conditions imposed upon the system and correlate these to bulk flow measurements.

1:15PM Q9.00011 Viscous flow and heat transfer in channels with structured walls, VLADIMIR AJAEV, Southern Methodist University, STEFFEN HARDT, PETER STEPHAN, Center of Smart Interfaces, TU Darmstadt — We develop a mathematical model of pressure-driven flow in channels with walls structured by arrays of parallel grooves filled with air or gas. Motivated by cooling applications, we study heat transfer from a heater embedded in the wall to the liquid. The flow in the liquid is described using a Stokes flow model, and thermocapillary effects due to presence of the liquid-gas interface segments in the grooves are also taken into account. The rate of heat transfer is determined by a competition of two physical effects: the insulating effect of the gas in the grooves, due to small thermal conductivity of the gas phase, and the reduction of the effective slip length at the channel wall due to the presence of the liquid-gas interface segments in the grooves. Criteria for heat transfer enhancement are formulated for different parameters of the structuring.

1:27PM Q9.00012 Utilizing an Automated Home-Built Surface Plasmon Resonance Apparatus to Investigate How Water Interacts with a Hydrophobic Surface, ADELE POYNOR, Allegheny College — By definition hydrophobic substances hate water. Water placed on a hydrophobic surface will form a drop in order to minimize its contact area. What happens when water is forced into contact with a hydrophobic surface? One theory is that an ultra-thin low-density region forms near the surface. We have employed an automated home-built Surface Plasmon Resonance (SPR) apparatus to investigate this boundary.

1:39PM Q9.00013 Quantification of slip at a liquid-solid interface – a novel approach¹, ALEKS PONJAVIC, MOURAD CHENNAOUI, JANET WONG, Imperial College — Much effort has been spent recently on experimentally proving the existence of interfacial slip of a Newtonian fluid. A constant limitation is the proximity to the surface at which the velocity of a fluid can be measured. A new technique is developed to maximise this proximity. The objective is to acquire velocity measurements of a fluid as close as possible to the liquid-solid interface while still using a direct method of observation. To ensure proximity to the surface the technique of photobleaching is adopted. Dye-doped water is pumped through a microfluidic channel. A short, intense pulse from a laser causes dye within the focal volume to bleach, creating a spot. The geometry of this spot evolves depending on the velocity profile of the fluid. By fitting the evolution of the spot with a Poiseuille velocity profile with slip the slip length is extracted. The hydrophobicity of the channel is varied by flowing silane through the channel prior to measurement, forming a self-assembled monolayer. Effects of shear rate and wettability on interfacial slip length are investigated.

¹This research is supported by an EPSRC grant.

1:51PM Q9.00014 Effects of Interfacial Translation-rotation Coupling for Confined Ferrofluids¹, ANGBO FANG, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay Road, Kowloon, Hong Kong — Ferrofluids have wide applications ranging from semiconductor fabrications to biomedical processes. The hydrodynamic spin diffusion theory for ferrofluids has been successful in explaining many experimental data, but it suffers from some fatal flaws. For example, it fails to predict the incorrect flow direction for a ferrofluid confined in a concentric cylinder channel in the presence of a rotating magnetic field. In this work we develop a method to establish the general hydrodynamic boundary conditions (BCs) for micro-polar fluids such as ferrofluids. Through a dynamic generalization of the mesoscopic diffuse interface model, we are able to obtain the surface dissipation functional, in which the interfacial translation-rotation coupling plays a significant role. The generalized hydrodynamic BCs can be obtained straightforwardly by using Onsager's variational approach. The resulted velocity profile and other quantities compares well with the experimental data, strikingly different from traditional theories. The methodology can be applied to study the hydrodynamic behavior of other structured fluids in confined channels or multi-phase flows.

¹The work is supported by a research award made by the King Abdullah University of Science and Technology.

Wednesday, March 23, 2011 11:15AM - 2:15PM – Session Q13 GSNP DFD: Glassy Systems and Jamming I D225/226

11:15AM Q13.00001 The Influence of Boundary Roughness on the Dynamics of Confined Colloidal Suspensions near the Glass Transition¹, DANIEL J. REAL, KAZEM V. EDMOND, ERIC R. WEEKS, Emory University — We study the relationship between boundary conditions and particle motion in confined, concentrated colloidal suspensions. Studies of polymer fluids in confinement have shown that changes in mobility are strongly dependent upon the polymer/surface interaction. We model this interaction by observing the effects of textured surfaces on colloidal particle mobility in confined dense suspensions (near the glass transition). We use high-speed confocal microscopy to directly image and track the colloidal particles in thin, wedge-shaped sample chambers made from textured glass. We texture the glass in a controlled, reproducible manner by spincoating and sintering colloidal suspensions onto glass slides. We expect the texturing to frustrate the formation of layers seen in smooth-walled confinement, resulting in decreased translational diffusion as compared to the smooth wall case. By studying these dynamics we gain a better understanding of the glass transition and its dependence on interfacial dynamics versus finite size effects.

¹Supported by NSF Grant No. DMR-0804174

11:27AM Q13.00002 Structural Rearrangements in Confined Colloidal Liquids under Oscillatory Shear, PRASAD SARANGAPANI, University of Notre Dame, ANDREW SCHOFIELD, University of Edinburgh, Y. ELAINE ZHU, University of Notre Dame — We have investigated the dynamics of confined suspensions under oscillatory shear using a micron-gap rheometer interfaced with confocal microscopy. Our system consists of sterically stabilized poly-(methyl methacrylate) (PMMA) particles suspended in density and refractive index matched solvents at particle volume fractions, $\phi = 0.40-0.43$, confined between two solid surfaces with gaps ranging from $\sim 10-30$ particle layers. Above a threshold strain of $\sim 6\%$ where an applied deformation is sufficient to induce plastic behavior, we find that structural rearrangements are highly anisotropic. Non-affine motion, determined by subtracting the globally uniform strain from the bare particle coordinates, reveals that particles move as cooperatively rearranging groups with a preferred orientation transverse to the flow direction. Measures which probe cooperative dynamics all reveal a strong amplitude, thickness, and directional dependence on the characteristic sizes of cooperatively rearranging regions. Interestingly, we find that medium range orientational order has a significant influence on shear-induced dynamics, particularly the shapes of rearranging regions.

11:39AM Q13.00003 Application of Edwards' statistical mechanics to polydisperse and high-dimensional jammed sphere packings, MAXIMILIEN DANISCH, Ecole Normale Supérieure de Cachan, YULIANG JIN, HERNAN MAKSE, The City College of New York, PATRICK CHARBONNEAU, Duke University, SAM MEYER, Université de Lyon, CHAOMING SONG, Northeastern University, FRANCESCO ZAMPONI, Ecole Normale Supérieure — The Edward's statistical mechanics of jammed sphere packings [Song et al., Nature (London) 453, 629 (2008)] is generalized to different systems: polydisperse sphere packings in three dimensions, and high-dimensional monodisperse sphere packings. The theory predicts the density of random close packing and random loose packing of polydisperse systems for a given distribution of particle size and describes packings for any interparticle friction coefficient. In the high-dimensional limit, an asymptotic solution of the self-consistent relation is obtained by saddle-point evaluation and checked numerically. The resulting random close packing density scaling is consistent with that of other approaches, such as replica theory and density-functional theory. The theory could serve as a starting point to solve more difficult problems: such as predicting the optimal density of non-spherical packings, and understanding the higher-order correlations present in amorphous jammed packings.

11:51AM Q13.00004 Cyclic simple shear in a two-dimensional granular system¹, JIE REN, JOSHUA DIJKSMAN, ROBERT BEHRINGER, Department of Physics, Duke University — We study the evolution of a 2D granular system consisting of frictional photo-elastic disks under large numbers of small-amplitude cyclic shear cycles. We are particularly interested in the reversibility of the system under cyclic shear. The experiments are carried out on a specially designed apparatus which can create quasi-static, nearly uniform simple shear. By using photo-elastic particles and a fluorescent labelling technique, we obtain information about displacement, rotation and contact forces for each particle following each small strain. We also obtain the system-level behaviour over many shear cycles. To better understand the nature of jamming, we have carried out shearing runs that explore various initial states which are initially unjammed, isotropically jammed or anisotropically jammed, and we compare the results for different initial states.

¹This work is supported by grants DMR09-06908, NSF 0835742, and ARO W911NF-07-1-1031

12:03PM Q13.00005 Microscopic Dynamics of Quasi-2D Dense Colloidal Gels¹, MATTHEW LOHR, ARJUN YODH, University of Pennsylvania — In this work, we investigate the microscopic dynamics of quasi-2D dense attractive colloidal systems. We confine bidisperse polystyrene spheres between glass coverslips in a suspension of water and 2,6-lutidine; as we increase the temperature of the sample into a critical regime, lutidine wets the colloids, creating a strong attractive interaction ($> 4kT$). We specifically study suspensions in the "dense gel" regime, i.e., at a volume fraction high enough that the attractive particles form a spanning cluster, yet just low enough that there exists some structural heterogeneity larger than the individual particle size. We track the particle locations via bright-field video microscopy and analyze the dynamics of the system in order to compare them to lower-volume-fraction gel states and higher-volume-fraction glassy states. In doing so, we pinpoint the similarities and differences in the mechanisms for dynamic arrest in low-density colloidal gels and high-density colloidal glasses.

¹ Supported by NSF Grant DMR-0804881, MRSEC Grant DMR-0520020 and NASA Grant NNX08AO0G.

12:15PM Q13.00006 Structural Correlations in Glass-Forming Hard Spheres Fluids, PATRICK CHARBONNEAU, Duke University, BENOIT CHARBONNEAU, St. Jerome's University and University of Waterloo — Recent studies have detected the presence of a growing static length scale associated with the glassy dynamical slowdown. Yet no fully satisfying microscopic description of such a length scale has yet been formulated. We critically evaluate the hypothesis that correlated structural defects could underlie the growing relaxation time in deeply supersaturated fluid. Though a clear structural signature of a developing order in these systems is found, the resulting defect geometry does not lead quite match the Frank- Kasper defect scenario. The dimensionally generalizable nature of the defects, however, make them promising options for defining static observables.

12:27PM Q13.00007 Study of experimental protocols for producing random close packed colloids, KELSEY HATTAM, ERIC R. WEEKS — A collection of spheres can be packed tightly into an amorphous state known as "random close packing." In our experiment, colloidal particles are allowed to slowly sediment forming a random close packed state. By adjusting the solvent's density we finely control the rate at which the sedimentation occurs. We then use confocal microscopy to image the sample. By imaging overlapping regions we determine the positions of hundreds of thousands of particles. From this data, we measure the distribution of Voronoi volumes and the contact number distribution, and examine how these distributions depend on the sedimentation rate.

12:39PM Q13.00008 Rotational and Translational Phonon Modes in Glasses Composed of Ellipsoidal Particles¹, PETER J. YUNKER, KE CHEN, University of Pennsylvania, ZEXIN ZHANG, Soochow University, WOUTER G. ELLENBROEK, Eindhoven University of Technology, ANDREA J. LIU, ARJUN G. YODH, University of Pennsylvania — The effects of particle shape on the vibrational properties of colloidal glasses are studied experimentally. 'Ellipsoidal glasses' are created by stretching polystyrene spheres to different aspect ratios and suspending the resulting ellipsoidal particles at high packing fraction. By measuring displacement correlations between particles, we extract vibrational properties of the ellipsoidal glass. Low frequency modes in glasses composed of ellipsoidal particles with major/minor axis aspect ratios ~ 1.1 are observed to have predominantly rotational character. By contrast, low frequency modes in glasses of ellipsoidal particles with larger aspect ratios (~ 3.0) exhibit a mix of rotational and translational character. All glass samples were characterized by a distribution of particles with different aspect ratios. Interestingly, even within the same sample it was found that small- aspect-ratio particles participate relatively more in rotational modes, while large-aspect-ratio particles tend to participate relatively more in translational modes.

¹We acknowledge financial support from the NSF through DMR-0804881, PENN MRSEC DMR-0520020, and NASA NNX08AO0G.

12:51PM Q13.00009 Dynamical heterogeneities and fluctuations of the time variables in structural glasses, KARINA E. AVILA, HORACIO E. CASTILLO, Ohio University, AZITA PARSAEIAN, Northwestern University — The existence of dynamical heterogeneities in disordered materials is considered now as a crucial element in explaining many observed features of their dynamical behavior. In this work, we investigate a possible hypothesis for their origin, which assumes that they emerge from soft (Goldstone) modes associated with a broken continuous symmetry under time reparametrizations. To test this hypothesis, we construct coarse grained observables from data obtained in simulations of four models of structural glasses. The fluctuations of these observables are decomposed into transverse components associated with the postulated time-fluctuation soft modes and a longitudinal component unrelated to them. We find that as temperature is lowered and timescales are increased, the time reparametrization fluctuations become increasingly dominant and their correlation volumes grow together with the correlation volumes of the dynamical heterogeneities, while the correlation volumes for longitudinal fluctuations remain small.

1:03PM Q13.00010 Experimental observation of deformation and structural defects in hard-sphere colloid glasses, KATHARINE JENSEN, Harvard University Department of Physics, NOBUTOMO NAKAMURA, Harvard University School of Engineering and Applied Sciences, DAVID WEITZ, Harvard University Department of Physics, Harvard University School of Engineering and Applied Sciences, FRANS SPAEPEN, Harvard University School of Engineering and Applied Sciences — We performed experiments on a 1.55- μm -diameter monodisperse, hard-sphere colloid glass under simple shear at various strain rates, while simultaneously tracking real-time individual positions of roughly 100,000 particles by confocal microscopy. We probe the elastic, anelastic, and plastic responses of the system to applied strain, with particular focus on identifying the local mechanisms of deformation. In plastic deformation, we observe thermally activated rearrangements of groups of particles, the nature and concentration of which are correlated with local parameters such as strain, Voronoi volume, and free volume.

1:15PM Q13.00011 Aging dynamics of a colloidal glass - time resolved viscoelastic properties and the role of flow history¹, CHINEDUM OSUJI, AJAY NEGI, Yale University — Many colloidal suspensions are inherently out of equilibrium and display a slow evolution of their dynamics over time. However, many features of the glass transition as encountered in polymer and molecular glasses are not conserved. This phenomenon is still not completely understood and little is known of the connection between flow history, as a determinant of the initial system state, and subsequent aging dynamics. Further, the changes in the energy landscape during aging can be understood from the frequency and strain dependence of the shear modulus but the non-stationary nature of these systems frustrates investigation of their instantaneous underlying properties. Here we discuss the use of stress jump experiments that investigate the role of flow history on aging, and the systematic reconstruction of the frequency and strain dependence as a function of age for a repulsive colloidal glass undergoing structural arrest and aging. We uncover a connection between the aging behavior and the rate of flow cessation that is additionally reflected in the dynamics of residual stress relaxation. Strikingly, the frequency dependence at fixed times can be rescaled onto a master curve, implying a simple connection between the aging of the system and the change in the frequency dependent modulus.

¹The authors acknowledge NSF funding under CBET-0828905.

1:27PM Q13.00012 Jamming, Clogging, and Fragility in Frictionless Disk Systems with Quenched Disorder, CHARLES REICHHARDT, Los Alamos National Laboratory, EVAN GROOPMAN, ZOHAR NUSSINOV, Washington University, CYNTHIA OLSON REICHHARDT, Los Alamos National Laboratory — We consider a two-dimensional simulation model of binary frictionless disks which have a well defined jamming density of $\phi_j \approx 0.84$ in the absence of quenched disorder. When quenched disorder is added in the form of impenetrable immobile disks, the jamming density is reduced. As the density of the quenched disorder sites increases, we observe a crossover from a jamming transition to a clogging transition. The clogged state is defined as a highly heterogeneous granular packing that resists shear along one direction and that is composed of a combination of high density patches at the clean jamming density and very low density patches or voids. These clogged states are fragile in the sense that they are only clogged in the direction of an externally applied drive. After a clogged state has formed, if a new drive is applied in a different direction the disks can flow freely for a period of time before reorganizing into a new clogged state. In contrast, jammed systems are jammed in all directions simultaneously.

1:39PM Q13.00013 Coupling Between Translational and Orientational Order in Fiber Suspensions¹, ALEXANDRE FRANCESCHINI, EMMANOUELA FILIPPIDI, Center for Soft Matter Research, New York University, ELISABETH GUAZZELLI, IUSTI-CNRS UMR 6595 - Polytech Marseille - Aix-Marseille University, DAVID PINE, Center for Soft Matter Research, New York University — Suspensions of non-Brownian fibers under a small oscillatory shear flow find a random but completely reversible state, called “random organization”: at each period, the non-hydrodynamic interactions modify both the orientation and positions of fibers, until a reversible configuration is found. As observed in sphere suspensions, there is a nonequilibrium absorbing phase transition when the strain is increased above a concentration-dependant threshold. The transient time, during which the activity decays algebraically, has a diverging duration; critical exponents are consistent with Manna universality class. Above the threshold, fibers get progressively aligned towards the vorticity and a reversible steady state is eventually found for a range of strain. This behavior is specific to fiber suspensions. We study whether or not these oriented reversible states are critical states. We experimentally evaluate the angles distribution of fibers in both vertical and horizontal planes and discuss the relation between these distributions and the existence of a reversible state.

¹Primarily funded by the MRSEC Program of the NSF under Award Number DMR-0820341

1:51PM Q13.00014 Force correlations near point J in a lattice model of jamming, SCOTT MILNER, JILLIAN NEWHALL, Penn State University — We have constructed a lattice model of a jammed system in $d = 2$ dimensions near the isostatic point (Point J). Adapting the Tighe model, we represent a jammed pack of particles as a regular hexagonal array, with repulsive forces between nearest neighbors. We generate near-isostatic jammed configurations by carrying out a Monte Carlo simulation with Tighe “wheel moves”, which rearrange forces locally while preserving force balance on every particle. (Wheel moves correspond to a small dilation of a given particle.) The MC simulation is progressively biased towards the creation of “missing contacts”, bonds which bear zero force. We reveal long-range correlations in the force network near Point J by determining for each particle the smallest “collective move” — a set of wheel moves that taken together dilates the given particle, while preserving the existing missing contacts. The size of these collective moves diverges as Point J is approached.

2:03PM Q13.00015 Time and volume fraction dependence of dynamic heterogeneity in a glass-forming binary hard-sphere mixture, ELIJAH FLENNER, GRZEGORZ SZAMEL, Colorado State University - Chemistry Department — We examined dynamic heterogeneity in a glass-forming binary hard-sphere mixture for volume fractions up to and including the so-called mode-coupling transition. We calculated the dynamic susceptibility $\chi_4(t)$, the four-point structure factor $S_4(q; t)$ and the dynamic correlation length $\xi(t)$. We find that the correlation length increases with time as $\xi(t) \sim \ln(t)$ and is independent of ϕ for times approximately between the β and α relaxation time. The dynamic length plateaus at a ϕ dependent value $\xi_{\max}(\phi)$. We find that $\xi_{\max}(\phi)$ is proportional to the dynamic length at the α relaxation time, $\xi(\tau_\alpha)$. Finally, while for a limited range of volume fractions $\xi(\tau_\alpha) \sim \tau_\alpha^{1/z}$ with $1/z \approx 0.2$, we find that $\xi(\tau_\alpha) \sim \ln(\tau_\alpha)$ describes our data well for all ϕ .

Wednesday, March 23, 2011 2:30PM - 5:30PM –
Session T9 DFD: Flow Instabilities, Turbulence and CFD D220

2:30PM T9.00001 ABSTRACT WITHDRAWN –

2:42PM T9.00002 Modal decomposition of free and forced circular jets at low and high Reynolds numbers, MURALIDHAR KRISHNAMURTHY, Professor, TRUSHAR GOHIL, doctoral student, ARUN SAHA, Assistant Professor — Free and forced jets are important in applications such as combustion, propulsion, mixing, and aero-acoustics. Jet control for noise reduction and mixing efficiency can be achieved by manipulating the flow structures. The most energetic structures of a flow field can be objectively recovered by proper orthogonal decomposition. POD extracts a basis for modal decomposition as eigenfunctions from an ensemble of signals. In the present work, the snapshot POD method is applied to data recorded from direct numerical simulation as well as large eddy simulation in three dimensions. Free jets are reported at a Reynolds number of 1000 and 10000 and 4300 for forced jets. Results show that all of the kinetic energy of laminar flow is stored in large-scale structures while for the turbulent jet, a broader distribution of kinetic energy is obtained. At $Re = 1000$, 40 snapshots of the flow field are adequate to resolve the major flow structures. For $Re=10000$, at least 100 snapshots are required for a good spectral representation. Blooming jets arising from dual mode forcing show the formation of odd-even pairs. The first pair contains the details of branching. In addition, the higher order modes capture the inherent jet instability mechanisms.

2:54PM T9.00003 Generalized Saffman-Taylor formula for multi-layer Hele-Shaw flows, PRABIR DARIPA, Texas A&M University — Stability theory plays a major role from fundamental science to applied sciences. It is useful in the design of many processes and engineering instruments as well as in explaining many phenomena. In this paper we review some of the author's and his collaborator's recent works on the extension of Saffman-Taylor instability which occurs at an interface between two immiscible fluids in porous media and Hele-Shaw cells when displacing fluid is less viscous than the displaced one. The growth rate of interfacial disturbances is given by a formula called Saffman-Taylor formula which plays a very important role in many areas including flows in porous media and oil recovery among many others. In this talk, we will present our results on the generalization of this formula to multi-layer flows involving many interfaces. As an application of the generalized Saffman-Taylor formula, we will derive necessary conditions for suppressing instability of two-layer flows by introducing arbitrary number of constant viscosity fluid layers in between. The important role that these conditions play in stabilization of hydrodynamic instabilities in Hele-Shaw flows will be discussed.

3:06PM T9.00004 The stability of a droplet suspended in a straight micro-channel, HAIDER HEKIRI, TAKUMI HAWA, School of Aerospace and Mechanical Engineering, The University of Oklahoma, Norman, OK 73019 — CFD simulations of the dynamics of a two-dimensional, incompressible, and two coupled spherical-cap water droplets suspended in a straight micro-channel, whose channel height is D , have been conducted to investigate the stability of the droplet. FLUENT with a 2-D pressure based solver is utilized in this simulation. The suspended droplet states are measured by the location of the center of mass of the droplet. We find that there is a critical volume, $V_c(D)$, where asymmetric droplet states appear in addition to the basic symmetric states when $V > V_c(D)$. Using the CFD it is demonstrated that when $V < V_c(D)$ the symmetric droplet states have a stable mode. However, when $V > V_c(D)$ the symmetric states become unstable and asymmetric states have a stable mode. The bifurcation of asymmetric states at $V_c(D)$ has a pitchfork nature. The simulations clarify the relationship between the linear stability results and the experimental results of the droplet behavior.

3:18PM T9.00005 Liquid-air interface instability due to an in-plane electric field, MIKHAIL PEVNYI, JAKE FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute - KSU — We report observations of an instability at the free surface of a liquid due to an in-plane electric field. The horizontal air-liquid interface in a partially filled sample cell between vertical electrodes exhibited first oscillations, then increasingly turbulent fluctuations as the strength of the horizontal electric field was increased. This behavior was observed in toluene and chloroform; the applied AC field was sinusoidal with $f=60\text{Hz}$. The dynamics of the interface was probed via dynamic light scattering. We present our experimental observations, as well as a simple model and numerical simulations of the interface dynamics under the influence of the applied electric field.

3:30PM T9.00006 Stretch-induced wrinkles in reinforced membranes, ATSUSHI TAKEI, ESPCI, FABIAN BRAU, Universit de Mons, BENOÎT ROMAN, JOSÉ BICO, ESPCI — We study through model experiments the buckling of a rigid stripe (or fiber) embedded in a soft membrane under compression. The compression is induced through Poisson effect when the membrane is stretched perpendicularly to the stripe. The wavelength of the wrinkles is found to depend on the material properties and the stretching strain. A balance between the bending and stretching energies of both the membrane and the stripes dictates this wavelength: $\lambda \sim (Bd / E_S H_S \delta)^{1/3}$, where B is the bending stiffness, d the width of the rigid band, δ the strain, and E_S and H_S the Young modulus and the thickness of the membrane, respectively. The characteristic extension of the wrinkled zone is set by the wavelength. This result also applies to fibers imbedded in a thin membrane. However, in-plane buckling is observed when the thickness of the membrane is large compared with the radius of the fiber. In this last regime, we find $\lambda \sim R(E_F / E_S)^{1/4}$, where E_F and R are the Young modulus and the radius of the fiber, respectively.

3:42PM T9.00007 Computational Parametric Study of R-M Instability Growth for an Inclined Interface¹, JACOB MCFARLAND, DEVESH RANJAN, Texas A&M University, JEFF GREENOUGH, Lawrence Livermore National Laboratory — An inclined interface perturbation is studied for an RM instability to model upcoming experiments in the Texas A&M inclined shock tube facility. Simulations were created using the ARES code developed at Lawrence Livermore National Lab. A parametric study was performed for inclination angles from 30 to 60 degrees, incident Mach numbers of 1.5 to 2.5, and high Atwood number gas pairs air-SF6 and helium/SF6. Qualitative results are examined to show the relative effects of these parameters. Interface growth rates are calculated and compared to the existing linear growth regime models. A new model is proposed based on the interface geometry and compared to the simulation results.

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

3:54PM T9.00008 Drop Splashing on a Smooth Surface at Low Velocities, CACEY STEVENS, SIDNEY NAGEL, University of Chicago — When a low viscosity liquid drop impacts on a smooth, dry surface, a thin fluid sheet is emitted which subsequently breaks up into a distribution of secondary droplets. Ambient gas pressure is crucial in creating this splash: splashing is completely suppressed below a threshold pressure [1]. There are several regimes that occur as the velocity and liquid viscosity are varied [2]. Here, we discuss splashing in the low velocity, low viscosity regime. We explore how the threshold pressure scales with drop size, as well as liquid viscosity. We also characterize the dependence of threshold pressure with molecular weight of the surrounding gas.

[1] L. Xu, S. Nagel, and W. Zhang. Phys. Rev. Lett. 94, 184505 (2005).

[2] L. Xu. Phys. Rev. E 75, 056316 (2007).

4:06PM T9.00009 Elastic effects on the shear flow instabilities in viscoelastic fluids, AHMED KAFFEL, Department of Mathematics Virginia Tech, DEPARTMENT OF MATHEMATICS VIRGINIA TECH TEAM, DEPARTMENT OF MATHEMATICS TEAM — A linear stability analysis was applied and the stability equation is derived and solved numerically using the spectral Chebyshev collocation method. The objective is to study the elastic effects on the instability of inviscid parallel shear flows. We focus on the upper convected Maxwell model in the limit of infinite Weissenberg and Reynolds numbers. Specifically, we study the effects of elasticity on the instability of a few classes of simple parallel flows, specifically plane Poiseuille and Couette flows, the hyperbolic-tangent shear layer and the Bickley jet. The algorithm is computationally efficient and accurate in reproducing the discrete eigenvalues. We consider flows bounded by walls as well as flows bounded by free surfaces. In the inviscid, nonelastic case all the flows we study are unstable for free surfaces. In the case of wall bounded flow, there are instabilities in the shear layer and Bickley jet flows. In all cases, the effect of elasticity is to reduce and ultimately suppress the inviscid instability. The numerical solutions are compared with the analysis of the long wave limit and excellent agreement is shown. We found flows which are long wave stable, but nevertheless unstable to wave numbers in a certain finite range. While elasticity is ultimately stabilizing, this effect is not monotone; there are instances where a small amount of elasticity actually destabilizes the flow.

4:18PM T9.00010 Thermal convection in multiphase systems, LUCA BIFERALE, University of Rome "Tor Vergata", PRASAD PERLEKAR, TUE, Eindhoven, MAURO SBRAGAGLIA, ANDREA SCAGLIARINI, University of Rome "Tor Vergata", FEDERICO TOSCHI, TUE, Eindhoven, ICTR COLLABORATION — We present preliminary results of a numerical study of two dimensional and three dimensional multiphase thermal convection close to the phase transition and in presence of phase coexistence. The numerical algorithm is based on a suitable implementation of multiphase Lattice Boltzmann scheme with non-ideal pressure tensor. We discuss the effects of droplets and bubbles formation on the global heat flux from bottom to top boundaries.

4:30PM T9.00011 Vortex Sheet Model for a Turbulent Mixing Layer, UJJAYAN PAUL, RODDAM NARASIMHA, MEHEBOOB ALAM, JNCASR, Jakkur, Bangalore 64 — The primary aim of this work is to study instability induced roll up of a slightly perturbed vortex sheet in an Euler fluid. A point vortex model tends to evolve into a chaotic cloud of point vortices instead of smooth double branched spirals. The present model uses linear splines to interpolate the vortex sheet. Computer simulation of this vortex sheet is numerically prohibitive. However, the evolution of the vortex sheet can be performed conveniently using a closed form equation of motion which derived from the basic equations of vortex dynamics. The vortex sheet rolls up into a smooth double branched spiral. A vortex core is formed by regular windings of the vortex sheet and irrotational fluid in between the layers. Various statistical quantities like the growth rate and mean velocity profiles are computed along with the evolution of the vortex sheet. The problem of spontaneous appearance of singularity in an evolving vortex sheet is treated in detail. The critical time for the present vortex sheet model is calculated analytically and compared to the numerical value.

4:42PM T9.00012 Nonlinear Deformation in Weak Turbulence¹, NICHOLAS OUELLETTE, DOUGLAS KELLEY, YANG LIAO, Department of Mechanical Engineering & Materials Science, Yale University — Turbulent and chaotic flows are well known to mix efficiently: by repeatedly stretching and folding material volumes, material lines stretch exponentially quickly and gradients of an advected scalar field can become very large. By adapting a technique originally introduced to study plasticity in glassy solids, we explicitly separate stretching (a linear transformation) from folding (a nonlinear transformation) in a quasi-two-dimensional experimental flow and study them independently. We compare results from two forcing schemes: one that is dominated by rotation, and another that is dominated by shear.

¹This work was supported by NSF Grant No. DMR-0906245.

4:54PM T9.00013 Principal Direction of Scalar Transport in Wall Turbulence¹, CHIRANTH SRINIVASAN, DIMITRIOS PAPAVALIIOU, The University of Oklahoma — Lagrangian scalar tracking in conjunction with direct numerical simulation is utilized in an infinitely long channel to study the principal direction of scalar transfer for both forwards and backwards single particle dispersion. Four regions are of interest: the viscous sub-layer, the transition region (between the viscous sub-layer and the logarithmic region), the logarithmic region and the center of channel. Fluctuating velocities of scalar markers released in the flow field are correlated forwards and backwards in time to find the components of the correlation coefficient tensor. Eigenvalues and eigenvectors are obtained for both the forwards and backwards dispersion and for fluids with Prandtl number between 0.1 and 1000. The largest eigenvalues are higher in the case of backwards dispersion compared to the case of forwards dispersion. The eigenvector inclinations relative to the yz plane are different for forwards and backwards dispersion (at times comparable to the Lagrangian timescale).

¹NSF under grant CBET-0651180.

5:06PM T9.00014 Molecular origins of continuum fluid mechanics: Atomic migrations of single-phase fluid and slip boundary conditions, ALAN GRAHAM, SHIHAI FENG, TONY REDONDO, Los Alamos National Lab — We report the results of molecular dynamics simulations of pressure-driven flows of liquid argon in circular and planar conduits. We find that in inhomogeneous shear flows the molecules migrate to the center of the conduits and establish large radial density gradients under conditions that were previously assumed to be incompressible. These are the first predictions of shear-induced migration in pure fluids subjected to inhomogeneous shear flows. These density gradients increase monotonically with Péclet number. They result in a blunted velocity profile that deviates from the parabolic profile predicted by the Navier-Stokes equations for an incompressible fluid. Comparisons with simulations where the flow exhibits zero or linear shear indicate that this phenomenon is the result of the nonlinear shear flows and the finite size of the molecules.

5:18PM T9.00015 Search for Euler Singularity using Vortex Filaments, SAHAND HORMOZ, MICHAEL BRENNER, Harvard University — A promising mechanism for generating a finite-time singularity in the incompressible Euler equations is stretching of vortex filaments. An exhaustive search of all possible initial conditions involving filaments, however, is not practically feasible. In this talk, I will show that two interacting vortex filaments can not generate a singularity for any initial conditions, by analyzing the asymptotic self-similar limit of their collapse. Essentially, our approach entails a separation of the dynamics of the filament shape, from the shrinking of its core. We solve for the dynamics using a self-similar ansatz and show that the core does not shrink fast enough for a self-consistent collapse. The similarity solution allows for many different collapse geometries, consistent with the tireless effort in the past of investigating new initial conditions. Potential for a singularity at higher number of filaments is also discussed.

Thursday, March 24, 2011 8:00AM - 11:00AM –
Session V9 DFD: Self Assembly | D220

8:00AM V9.00001 Effects of cluster diffusion on the island density and size-distribution in submonolayer island growth

, YEVGEN KRYUKOV, JACQUES AMAR, University of Toledo — The effects of cluster diffusion on the submonolayer island density and island-size distribution (ISD) $N_s(\theta)$ (where $N_s(\theta)$ is the number of islands of size s at coverage θ) are studied for the case of irreversible submonolayer growth of compact islands on a 2D substrate. In our model, monomers are deposited with deposition rate F while the mobility D_s of an island of size s satisfies $D_s \sim s^{-\mu}$. Results are presented for $\mu = 1/2$ (corresponding to Brownian motion) as well as for higher values of μ . In general, we find that the exponents describing the flux-dependence of the island and monomer densities vary continuously as a function of μ . For $\mu < 1$ we also find that the ISD exhibits power-law behavior up to a cross-over size S_c . However, the values of the corresponding exponents are significantly larger than previous theoretical predictions. A generalized scaling form for the ISD for $\mu < 1$ is also proposed which leads to excellent scaling of the entire distribution. In contrast, for $\mu \geq 1$ we find that, due to a competition between size-scales, neither our generalized scaling form nor the standard scaling form $N_s(\theta) = \theta/S^2 f(s/S)$ (where S is the average island-size) lead to scaling of the entire ISD. Instead, the scaled ISD becomes more sharply peaked with increasing D_1/F and coverage. This is in contrast to models with limited cluster mobility for which good scaling occurs over a wide range of coverages and D_1/F .

8:12AM V9.00002 Rate-equation approach to irreversible island growth with cluster diffusion

, BRADLEY HUBARTT, YEVGEN KRYUKOV, JACQUES AMAR, University of Toledo — A self-consistent rate-equation (RE) approach to irreversible island growth and nucleation is presented which takes into account the effects of cluster mobility. As a first application we consider the irreversible growth of compact islands on a 2D surface in the presence of monomer deposition (with rate F) and monomer diffusion (with rate D_1) while the mobility of an island of size s is assumed to satisfy $D_s = D_1 s^{-\mu}$ where $\mu \geq 0$. For coverages up to the peak island-density, we find excellent agreement between our RE and simulation results for the dependence of the island-density $N(\theta)$ on coverage θ for all values of μ considered, ranging from $\mu = 1/2$ (Brownian motion) to $\mu = \infty$ (immobile clusters). For $\mu \leq 2$, excellent agreement is also found between our simulation and RE results for the island-size distribution (ISD), while for higher values of μ the effects of correlations become important. We also demonstrate that the discrepancies between recent theoretical predictions for the exponents $\tau(\mu)$ and $\zeta(\mu)$ describing the size-dependence of the ISD for $\mu < 1$ and simulations can be explained by the geometry of compact islands. Our self-consistent RE approach may also be generalized to higher dimensions as well as to an arbitrary dependence of the cluster mobility on island-size.

8:24AM V9.00003 Kinetics and Thermodynamics of the Association of DNA Coated Colloids

, KUN-TA WU, FENG LANG, Center for Soft Matter Research, New York University, RUOJIE SHA, Chemistry Department, New York University, REMI DREYFUS, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn UMI 3254, NADRIAN SEEMAN, Chemistry Department, New York University, PAUL CHAIKIN, Center for Soft Matter Research, New York University — We have investigated the aggregation kinetics and thermodynamics of complementary DNA coated particles as a function of DNA coverage. The streptavidin on our particles can accommodate 69800 biotinylated DNA which has 50 base pair double strands and 11 base sticky ends. For full 100% coverage, the melting temperature, T_m , is 50.3 C. The transition width, ΔT , is 0.8 C, and the characteristic aggregation time, τ , is 4 minutes. For 2.5% (40 times less) coverage $T_m = 22$ C, $\Delta T = 5$ C, and $\tau = 11$ hours. A simple model which takes into account the number of DNA bonds and the multiplicity of their arrangements accounts for the full time and temperature dependence of the particle aggregation.

8:36AM V9.00004 DNA driven 2D Assembly of Nanoparticles on Lipid Surfaces

, SUNITA SRIVASTAVA, DMYTRO NYKYPANCHUK, OLEG GANG, Brookhaven National Laboratory, Upton, NY, 11973 — Use of biomolecular linkers such as DNA due to its sequence-specific hybridization properties provides a versatile platform for assembly of nanoscale components. Here we investigated the DNA-based self-assembly of gold nanoparticles in 2D using lipid layer as fluid substrate. We examined the effect of lipid composition by vary the fraction of cationic and zwitterion lipids on formation of a particle monolayer. Using in-situ X-ray reflectivity we observed adsorption of DNA functionalized nanoparticles on charged lipid surfaces. The surface density of the particle monolayer can be tuned by changing the electrostatic interaction between the particles and the lipid surface. The in-situ measured particle desorption from the lipid surface due to a change of a salt concentration provides quantitative information on particle-surface interactions. The ex-situ studies on samples using XPS under similar conditions support our observations. Our studies explore the possibility to form regulated 2D systems, as well as provide basic understanding of interactions of charge nano-objects with lipids, which is important for the biomedical applications.

8:48AM V9.00005 Computational Analysis of DNA-Mediated Crystallization of Binary Colloidal Superlattices

, TALID SINNO, RAYNALDO SCARLETT, MARIE UNG, JOHN CROCKER, University of Pennsylvania — Colloidal self-assembly provides a potential avenue for the design of novel devices with unique optical and structural properties. Colloidal systems also provide useful insights into fundamental mechanisms of phase transitions such as crystal nucleation, growth and melting that are otherwise difficult to probe in atomic systems. A promising approach for realizing highly tunable colloidal assembly is to graft single-stranded DNA oligomer brushes onto the surfaces of particles in order to create attractive interactions between them. Using this approach, micro- and nanoscale particles have now been successfully assembled into several crystalline phases, including ordered, binary superlattice structures. Here, we apply Monte Carlo simulations and free energy calculations to generate a detailed picture for the assembly binary superlattice crystals. The interparticle potential used to perform the calculations was generated specifically for DNA-mediated interactions and verified by measurements. We develop a pseudo-phase diagram for the binary superlattice system which includes both thermodynamic and kinetic influences. The predictions of the pseudo-phase diagram are validated using direct simulations of crystal nucleation. Finally, we discuss recent findings related to diffusionless transformations in growing superlattice crystals that may be important in experiments aimed at growing these structures.

9:00AM V9.00006 DNA Linker Mediated Assembly of Gold Nanoparticles Superlattice¹

, HUIMING XIONG, CFN, BNL & Shanghai Jiao Tong University, MATTEW Y. SFEIR, CFN, BNL, DANIEL VAN DER LELIE, Biology Department, BNL, OLEG GANG, CFN, BNL — A BCC (body-centered-cubic) crystalline phase forms when flexible ssDNA linkers are added to the mixture of two types of dispersed, ssDNAs capped gold nanocolloids which are mutually non-complementary but complementary to the respective ends of the linker DNA. The state diagram of DNA linker mediated nanoparticle assemblies has been experimentally investigated and constructed by using in-situ small angle x-ray scattering. The optically active three-dimensional superlattice containing plasmonic particles and DNA-encoded chromophores were further fabricated using this approach. We investigated structural tunability and corresponding optical response of the multicomponent superlattices.

¹Support from the U. S. DOE Office of Science and Office of Basic Energy Sciences under contract No. DE-AC-02-98CH10886 and Shanghai Pujiang Program (10PJ1405400) is appreciated.

9:12AM V9.00007 Directed Self-Assembly of Colloidal Particles

, ZORANA ZERAVCIC, School of Engineering and Applied Sciences, Harvard University, JESSE COLLINS, Department of Physics, Harvard University, VINOTHAN MANOHARAN, School of Engineering and Applied Sciences, Harvard University and Department of Physics, Harvard University, MICHAEL BRENNER, School of Engineering and Applied Sciences, Harvard University — In nature, simple constituents like atoms, molecules and polymer chains, spontaneously organize into larger, higher order structures. Interactions involved in this self-assembly act on a local level. These facts inspire experimental and theoretical engineering of components able to organize into pre-designed complex systems. We perform numerical simulations of collections of DNA coated colloidal particles. We test different design rules for self-assembly with short-range interactions and explore the stability of equilibrium structures.

9:24AM V9.00008 Replication of nanoscale DNA patterns¹, CORINNA MAASS, TONG WANG, RUOJIE SHA, MIRJAM LEUNISSEN, REMI DREYFUS, NADRAN SEEMAN, PAUL CHAIKIN — We present an artificial supramolecular system mimicking self-replication and information transmission strategies in nature, but without the aid of enzymes or equivalent biological mechanisms. Using DNA nanotechnology techniques, we can make DNA tiles with selective interactions based on complementary single-strand connections. A linear tile pattern distinguished by their connector sequences is transmitted to a subsequent generation of copies by connector hybridisation. Longitudinal pattern formation and transverse copy attachment are well separated by different melting temperatures. We have achieved a faithful transmission of the pattern information to the second replication generation. We use AFM imaging to test for pattern fidelity and gel electrophoresis for quantitative yield analysis.

¹supported by a DAAD postdoc grant

9:36AM V9.00009 Designing colloids for alignment, REMI DREYFUS, CNRS, Compass Lab, TYCHO SLEATOR, NYU, KENNY MAYORAL, THOMAS G. MASON, UCLA, PAUL M. CHAIKIN, NYU — Inducing the spontaneous association of microscopic building blocks into macroscopic structures has been a promising way to create new materials for a variety of useful applications. Such fabrication processes typically require interactions between microscopic building blocks. The interactions that govern the assembly of these microscopic building blocks: electrostatic, magnetic, Van der Waals, depletion, and DNA interactions, are all currently being investigated. For all these cases, the attractive energy between the particles is proportional to the overlapping surface between the colloids. Controlling the positions and orientations of the microscopic building blocks is a critical issue in such processes. To date there has been no efficient or reliable process that enables such spontaneous assembly of building blocks. For the successful alignment of any particles that we desire to self-assemble, a shape with unique physical and mathematical properties must be identified. Under the assumption that energy is reduced in proportion to area overlap, we present a geometrical shape which, when encountering a similar shape from any initial configuration, is forced into a single relative orientation maximizing the overlap. The unique minimum of energy in the energy landscape drives the particles to self-assemble in a controlled orientation.

9:48AM V9.00010 Self-assembly of Nanoparticles into Planar Modulated Superstructures, MICHAEL ENGEL, University of Michigan — The advance in the synthesis of nanoparticles and colloids opens up the possibility to use them as building blocks for self-assembling novel materials. Ordered structures are especially interesting because they have unique photonic and electronic properties. Among the most complex ordered phases are commensurately and incommensurately modulated crystals. Although frequently found on the atomic scale in the bulk and as ordered structures of noble gases in adsorbed layers, modulated phases have so far not been known to self-assemble with nanoparticles. Here, we use computer simulations to study a two-dimensional system characterized by a simple isotropic interaction that could be realized in future with building blocks on the nanoscale. We find that the particles arrange themselves into planar hexagonal superstructures whose superlattice vector can be tuned reversibly by changing the temperature. Thermodynamic stability is confirmed by calculating the free energy with a combination of thermodynamic integration and the Frenkel-Ladd method. Different contributions to the free energy difference are discussed.

10:00AM V9.00011 Programmable, directed assembly of micron-scale components, CASPAR FLO-RYAN, ROBERT WESTERVELT¹, Harvard University — Self assembly is a nascent paradigm for assembling components in the micron to millimeter size range. Such assemblies are often performed by modifying the surface chemistries of the individual components or by creating flow fields directing them into position. We propose a method of directed assembly using dielectric contrast between the components and a surrounding fluid. A hybrid integrated-circuit / microfluidic device² will be used to trap and manipulate pieces into pre-defined patterns. The device contains an array of electrically-chargeable pixels on its surface, with a resolution of 10 μm .

¹PI

²Thomas Hunt, David Issadore, Robert Westervelt “Integrated Circuit/Microfluidic Chip to Programmably Trap and Move Cells and Droplets with Dielectrophoresis” *Lab on a Chip* 8, 81-87 (2008)

10:12AM V9.00012 Synthesis and Evaporative Self-Assembly of Polystyrene Nanotubes under Confinement, LU ZHANG, JODIE LUTKENHAUS, Texas A&M University, TEXAS A&M UNIVERSITY TEAM — Synthesis and manipulation of anisotropic building blocks into ordered structures has attracted increasing attention in recent years as nanowires and nanotubes (NWs/NTs) show great potential in many emerging technologies such as novel electric devices, optical units and biosensors. Here we use evaporation to align polystyrene NWs/NTs into distinct and interesting patterns. We synthesized polystyrene (PS) NWs/NTs of varied aspect ratio using anodic aluminum oxide (AAO) templates (200 nm pore size) using a melt-wetting technique. The template was removed, and NWs/NTs of controllable length ranging from several hundred nanometers to a few micrometers were released from the bulk PS film under ultrasonication. We further investigate the evaporative self-assembly of the synthesized polystyrene NTs under confined and “open” geometries and observe the alignment and assembled structures of the polystyrene NTs using scanning electron microscopy. Confocal laser scanning microscopy was also used to monitor the kinetics of the alignment process during evaporation. Results indicate that many factors (solvent, aspect ratio) contribute to the degree of NW/NT alignment relative to the evaporation front.

10:24AM V9.00013 Dynamic self-assembly of chemically-propelled nanoscale building blocks, YANPING CHEN, YUNFENG SHI, Rensselaer Polytechnic Institute — Self-assembly technique offers spontaneous, massively-parallel structure formation from bottom-up. So far, most research efforts have been focused on static self-assembly that is thermally driven towards a thermodynamic equilibrium. Less attention has been paid to dynamic self-assembly that evolves to a non-equilibrium steady state under a dissipative driving force. This project aims to investigate the non-equilibrium self-assembly behaviors of chemically-propelled nanoscale building blocks via molecular dynamics simulations. We utilize a catalytic building block, that has been shown, when isolated, to exhibit self-motile behavior when immersed in a fuel environment. Upon increasing the number density of the building blocks, interesting collective behaviors emerge due to direct interactions between the building blocks or indirect interactions via the fuel environment. The simulation system is also subjected to an artificial operation of converting products back to fuel molecules. The heat generated by the exothermic chemical reaction will also be removed. In this way, a steady-state, as well as the resulting dynamic self-assembly pattern, can be obtained.

10:36AM V9.00014 Dynamic Self-Assembly and Self-Propulsion in Nonequilibrium Magnetic Colloidal Ensembles at a Liquid/Liquid Interface¹, ALEXEY SNEZHKO, IGOR ARANSON, Argonne National Lab — Ensembles of interacting particles subject to external periodic energy fluxes often develop nontrivial dynamics. Magnetic colloidal particles suspended over an interface of two immiscible liquids and energized by vertical alternating magnetic fields give rise to novel dynamic self-assembled structures (“asters”) which are not accessible at the liquid/air interfaces. Ferromagnetically ordered nickel spherical particles have been used in our experiments. Novel structures are attributed to the interplay between surface waves, generated at the liquid/liquid interface by the collective response of magnetic microparticles to the alternating magnetic field, and hydrodynamic fields induced in the boundary layers of *both* liquids forming the interface. Two types of magnetic order is reported. We show that self-assembled aster structures become distorted in the presence of a small in-plane dc magnetic field and develop self-propulsion. The speed of locomotion can be effectively tuned by the amplitude of the dc field.

¹The research was supported by the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under the Contract No. DE AC02-06CH11357

10:48AM V9.00015 A Tunable Terahertz Detector Based On Self Assembled Plasmonic Structure on a GaAs 2DEG, CHE JIN BAE, DEEPU GEORGE, ROHIT SINGH, ANDREA MARKELZ, SUNY at Buffalo — Recently compact frequency sensitive THz detection has been achieved using gated gratings on 2DEG structure. The method is based on the resonant absorption of the 2D plasmon dependence on system dimension and the tunability of that dimension by depletion gating. Here we attempt to improve detector sensitivity, tunability and remove polarization dependence through the development of a gated grid design. The requirement for imaging applications of device dimensions on the order of < 1 micron over a detector area of 4 mm², suggest that standard lithographic approaches will be too costly for large scale detector production. Here we realize the gated grid plasmonic structure on 2DEG material by using nanosphere self assembly lithography. This fabrication method has not been widely developed for III-V processing but allows us to achieve large area sensitive detectors with tunability in the 1-4 THz range. In this paper we will discuss the fabrication method and characterization of the devices as a function of gate bias and temperature using FTIR and THz time domain measurements.

Thursday, March 24, 2011 8:00AM - 10:48AM —
Session V13 GSNP DFD: Glassy Systems and Jamming II D225/226

8:00AM V13.00001 Phonon Spectra in Disordered Clusters of Colloidal Particles with Attractive Interactions¹, ARJUN G. YODH, PETER J. YUNKER, KE CHEN, University of Pennsylvania, ZEXIN ZHANG, Soochow University — The influence of size and morphology on the vibrational properties of disordered clusters of colloidal particles with attractive interactions is studied experimentally. Water-lutidine mixtures induce fluid mediated attraction between micron-sized polystyrene particles, leading to the formation of attractive glasses with high local packing fractions. By measuring displacement correlations between particles, we extract the vibrational properties of these disordered clusters. Surprisingly, the spectra and character of vibrational modes did not depend on the number of particles involved. Rather, it depended strongly on the average number of nearest neighbors. An increase in the number of nearest neighbors shifted the phonon spectrum to higher frequencies, independent of the total number of particles in the cluster. Simulations of structureless random networks of springs support these results, and further suggest that the dependence of phonon spectrum on number of nearest neighbors is a generic property of disordered networks.

¹We acknowledge financial support from the NSF through DMR-0804881, the PENN MRSEC DMR-0520020, and NASA NNX08AO0G.

8:12AM V13.00002 Dynamics of Small-Molecule Glass Formers Confined in Nanopores¹, TIMOTHY PRISK, Indiana University Department of Physics, MADHUSUDAN TYAGI, NIST Center for Neutron Research, PAUL SOKOL, Indiana University Department of Physics — We report a comparative neutron scattering study of the molecular mobility and non-exponential relaxation of three structurally similar glass-forming liquids (isopropanol, propylene glycol, and glycerol) in bulk and confined in porous Vycor glass. Confinement reduces molecular mobility in all three liquids, and suppresses crystallization in isopropanol. High-resolution quasi-elastic neutron scattering spectra were fit to Fourier transformed Kohlrausch functions $\exp[-(t/\tau)^\beta]$, describing α -relaxation. The stretching parameter β is roughly constant with wavevector Q and temperature. Average relaxation times $\langle\tau(Q)\rangle$ are longer at lower temperatures and in confinement. They obey a power law $\langle\tau(Q)\rangle \propto Q^{-\gamma}$, where the exponent γ is modified by both temperature and confinement. Comparison of the bulk and confined liquids lends support to the idea that structural and/or dynamical heterogeneity underlies the non-exponential relaxation of glass-formers, as widely hypothesized in the literature.

¹This work was prepared under award 70NANB5H1163 from NIST, U.S. Department of Commerce. We acknowledge the support of NIST in providing the neutron research facilities used in this work.

8:24AM V13.00003 ABSTRACT WITHDRAWN —

8:36AM V13.00004 Emergence of rigidity at the dynamic glass transition: a replica approach calculation¹, GRZEGORZ SZAMEL, ELIJAH FLENNER, Department of Chemistry, Colorado State University — According to the mean-field replica theory of the glass transition, at the so-called dynamic transition the relaxation stops and the liquid freezes into one of many metastable states. We identify Goldstone modes of the resulting amorphous solid and derive a formal expression for its shear modulus. This expression is complementary to the formula used by Yoshino and Mezard [Phys. Rev. Lett. **105**, 015504 (2010)]. We combine our formal expression with the recently proposed version of the replica approach [G. Szamel, Europhys. Lett. **91**, 56004 (2010)] to calculate the shear modulus.

¹We gratefully acknowledge the support of NSF Grant CHE 0909676.

8:48AM V13.00005 Experimental study of dynamic rearrangements in repulsive and attractive glasses, ZEXIN ZHANG, Soochow University, PETER YUNKER, University of Pennsylvania, PIOTR HABDAS, Saint Joseph's University, ARJUN YODH, University of Pennsylvania — The influence of interparticle attraction versus repulsion on heterogeneous glass dynamics is explored with colloidal particles suspended in water-lutidine mixtures. The mixtures permit interparticle potentials to be tuned in situ from short-range repulsive to short-range attractive. Thus, a direct comparison of colloidal glass dynamics in samples composed of the same particles at the same volume fraction is possible. In both types of glasses, dynamics are found to be heterogeneous, and particles rearrange in a cooperative manner. By comparison to repulsive glasses, attractive glasses exhibit dynamics that are heterogeneous over a wider range of time and length scales, and involve more particles. Clusters of rearranging particles form string-like structures in repulsive glasses, and more compact clusters in attractive glasses. The experiments demonstrate explicitly that interparticle interactions affect glass dynamics.

9:00AM V13.00006 A family of systematically softened glass-formers, ZANE SHI, PABLO DEBENEDETTI, FRANK STILLINGER, Princeton University — We present a computational study of a family of binary glass-forming mixtures that interact via the generic $U = 4\epsilon[\lambda(\sigma/r)^n - \alpha(\sigma/r)^6]$, where $n = 7, 8, 9, 10, 11, 12$. λ and α are chosen such that the location and depth of the potential minimum are constant across all members of the family. We investigate the effects of softening on thermodynamic quantities such as energy and entropy, as well as dynamic properties such as diffusion and scattering. We also investigate the effects of softening on the energy landscape. In spite of the imposed constraint on well depth and location, we find profound effects of softening on all aspects of liquid and glassy behavior. The stability of the glasses is greatly enhanced by softening (soft liquids make hard glasses), and the relaxation rates in the corresponding liquids increase markedly upon softening. We present a comprehensive analysis of kinetic and thermodynamic fragilities in this family of glass-formers.

9:12AM V13.00007 Low-Frequency Vibrational Modes and Rearrangements in a Colloidal Glass Subject to Point Expansion¹, KEVIN APTOWICZ, MATTHEW COLAGRECO, RYAN MARGOLIS, West Chester University, PETER YUNKER, KE CHEN, ARJUN YODH, University of Pennsylvania — We conduct experiments on two-dimensional packings of colloidal thermosensitive hydrogel particles. The packing fraction of the colloidal suspension is tunable from liquid to deeply jammed by varying the global temperature of the sample. In addition, by tightly focusing an infrared laser on the sample, point expansion of the colloidal glass is induced via thermophoretic forces. We utilize displacement correlation matrix techniques employed in recent papers, and we employ video microscopy to derive the vibrational modes. The response of the sample to induced point expansion is analyzed over a range of packing fractions, with particular focus on the correlation between quasi-localized low-frequency vibrational modes and regions of rearrangements.

¹This research is supported by an award from Research Corporation (KBA), MRSEC grant DMR-0520020 (AGY), NSF grant DMR-0804881 (AGY), and NASA grant NNX08AO0G (AGY).

9:24AM V13.00008 Crystallization of the Lewis-Wahnström ortho-terphenyl model, ULF PEDERSEN, UC Berkeley, TOBY HUDSON, PETER HARROWELL, School of Chemistry, University of Sydney — Crystallization is observed during long molecular dynamics simulations of bent trimer molecules - one of the standard models in computational studies of viscous supercooled liquids. The crystal was not anticipated, but is surprisingly simple: the three spheres that make up the rigid molecule sit near the sites of a body centered cubic lattice (the trimer bond angle being almost optimal for this structure). Interestingly, the crystal exhibits orientational disorder with molecules aligned randomly along the three Cartesian axis (an example of cubatic orientational order). While crystallization does not disqualify this model for viscous dynamics studies (it may even be valuable that the crystal is known), it illustrates the stubborn ingenuity of molecules to pack in periodic structures and questions our intuition to predict such structures. Finally, this is a rare example of crystallization of a molecular model from melt.

9:36AM V13.00009 Vitrification of a monatomic simple liquid in two dimensions¹, TAKASHI ODAGAKI, Tokyo Denki University, TOMOKO MIZUGUCHI, Kyushu University — We investigate vitrification and crystallization process of a monatomic system by molecular dynamics simulation, where atoms interact via Lennard-Jones-Gauss potential. We first determine the time-temperature-transformation diagram by observing the crystallization time of the rapidly quenched state from the melt. The crystallization time becomes shortest at a certain temperature T^* . The glassy state at low temperatures is shown to be fairly long-lived. In order to examine atomic mechanism of the crystallization, we introduce a modified incoherent intermediate scattering function which measures the structural correlation to a target structure. We show that the crystallization above and below T^* take different paths. We also determine the free energy landscape (FEL) and show that the atomic dynamics is consistent with the FEL picture of the glass transition.

¹This work was partially supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports and Culture.

9:48AM V13.00010 Time reparametrization symmetry in a structural glass model, GCINA MAVIM-BELA, HORACIO E. CASTILLO, Ohio University, CLAUDIO CHAMON, Boston University, LETICIA CUGLIANDOLO, Université Pierre et Marie Curie - Paris VI — We explore the existence of time reparametrization symmetry in a particle system with quenched disorder. The system's density fluctuations are described by a stochastic equation (D. S. Dean, J. Phys. A:Math. Gen **29**, L613 (1996)). Using the Renormalization Group (RG) on the Martin-Siggia-Rose generating functional, we analytically probe the long time dynamics by systematically integrating over short time scale fluctuations. We find that the RG flow converges to a fixed point that is invariant under reparametrizations of the time variable.

10:00AM V13.00011 Viscosity, Shear Waves and Atomic Level Stress Correlations¹, VALENTIN LEVASHOV, JAMES MORRIS, TAKESHI EGAMI, University of Tennessee and Oak Ridge National Laboratory — The Green-Kubo equation relates the macroscopic stress-stress correlation function to a liquid's viscosity. The concept of the atomic level stresses allows the macroscopic stress-stress correlation function in the equation to be expressed in terms of the space/time correlations between the atomic level stress-stress correlation functions. Molecular dynamics studies show surprisingly long spatial extension of stress-stress correlations and also longitudinal and transverse waves propagating in liquids over ranges exceeding the system size. The results reveal that the range of propagation of shear waves corresponds to the range of distances relevant for viscosity. Thus our results show that viscosity is a fundamentally non-local quantity. We also show that periodic boundary conditions play very non-trivial, previously undiscussed, role in molecular dynamics simulations effectively masking the long range nature of viscosity.

¹This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences.

10:12AM V13.00012 Study of the de Almeida-Thouless line using power-law diluted one-dimensional Heisenberg spin glasses¹, AUDITYA SHARMA, PETER YOUNG, University of California at Santa Cruz — In a recent study, we showed that in mean-field theory, there is a de Almeida-Thouless (AT) line, that separates the low-temperature, low-field spin-glass phase from a high-temperature, high-field paramagnetic phase, for arbitrary m -component vector spin glasses, provided one applies a magnetic field that is *random in direction*. Building on this piece of work, here, we investigate whether or not there is an AT line beyond mean-field theory for Heisenberg spin glasses by performing Monte Carlo simulations on a power-law diluted one-dimensional Heisenberg spin glass for very large system sizes.

¹NSF

10:24AM V13.00013 Renormalization group analysis of the random first order transition, CHIARA CAMMAROTA, GIULIO BIROLI, IPhT, CEA/DSM-CNRS/URA 2306, CEA, Saclay France, MARCO TARZIA, GILLES TARJUS, LPTMC, CNRS-UMR 7600, Université Pierre et Marie Curie, Paris — We consider the approach describing glass formation in liquids as a progressive trapping in an exponentially large number of metastable states. To go beyond the mean-field setting, we provide a real-space renormalization group (RG) analysis of the associated replica free-energy functional. The present approximation yields in finite dimensions an ideal glass transition similar to that found in mean field. However, we find that along the RG flow the properties associated with metastable glassy states, such as the configurational entropy, are only defined up to a characteristic length scale that diverges as one approaches the ideal glass transition. The critical exponents characterizing the vicinity of the transition are the usual ones associated with a first-order discontinuity fixed point.

10:36AM V13.00014 Influence of pressure on fast relaxation in glass-forming materials, VLADIMIR NOVIKOV, University of Tennessee, Chemical Department, 1420 Circle Dr., TN, 37996, LIANG HONG, ALEXANDER KISLIUK, Oak Ridge National Laboratory, Oak Ridge, TN 37831, ALEXEI SOKOLOV, University of Tennessee, Chemical Department, 1420 Circle Dr., Knoxville, TN, 37996 — The spectra of GHz-THz dynamics in glass forming materials have two main contributions: the boson peak and the fast relaxation that overlaps with the low-frequency flank of the boson peak. The nature of both contributions remains a subject of active discussions. Applying pressure helps to separate the temperature and volume effects on the fast dynamics. Although the boson peak under pressure was investigated recently by several groups, less attention was devoted to the fast relaxation. In this work we present the study of the fast relaxation measured in some molecular and polymeric glass formers under pressure by light (Raman and Brillouin) scattering. Different experimental conditions were applied: isothermal, isobaric, isokinetic, and isochoric. The results are analyzed within the frames of various theoretical models. In particular, we check in detail the predictions of the soft-potential model of glassy dynamics.

Thursday, March 24, 2011 11:15AM - 2:15PM –
Session W9 DFD: Self Assembly II followed by Vesicles and Micelles II D220

11:15AM W9.00001 Self-assembly of two-dimensional systems with off-center core-corona architecture, DANIEL SALGADO, CARLOS MENDOZA, Instituto de Investigaciones en Materiales, UNAM — Physical systems with core-corona architecture, such as dendritic polymers or hyper-branched star polymers which are characterized by two repulsive length scales, related to the hard and soft repulsions, respectively, show the spontaneous formation of stripe phases. Here we study, by using Monte Carlo simulations, how robust is the stripe formation process upon a shift in the center of the core with respect to the corona in a two-dimensional system of colloidal particles. We find that for sufficiently large shifts, the strip phases are replaced by a sort of plastic (or glassy) colloidal crystal consisting of a regular lattice of coronas inside of which disordered aggregates of cores coexist. The model investigated in this work could be useful for the design of colloidal plastic crystals.

11:27AM W9.00002 Limit of validity of Ostwald's rule of stages in a model of solution crystallization¹, LESTER HEDGES, STEPHEN WHITELAM, Molecular Foundry, Lawrence Berkeley National Laboratory — Many systems take “nonclassical” crystallization pathways, forming ordered solids via intermediates that do not share the architecture of the stable material. We possess only rules-of-thumb to explain such dynamics. Chief among them is Ostwald's rule of stages, which states that the phase that first emerges is the one closest in free energy to the parent phase. Although widely applicable, the rule breaks down in many experiments and computer simulations. It is therefore clear that the rule is without firm theoretical foundation, but it is not clear when it should apply. To this end we test Ostwald's rule of stages in a lattice model of solution crystallization. We find that rule holds in certain regions of parameter space and breaks down in others. We argue that its breakdown can be predicted using simple arguments. In addition, we find that crystallization pathways depend qualitatively on both the thermodynamic landscape prescribed by inter-particle interactions and on the relative rates of particle rotations and translations.

¹Supported by the Center for Nanoscale Control of Geologic CO₂, a U.S. D.O.E. Energy Frontier Research Center, Contract No. DE-AC02-05CH11231.

11:39AM W9.00003 Mesophase behavior and rheology of polyhedral particles¹, UMANG AGARWAL, FERNANDO ESCOBEDO, School of Chemical and Biomolecular Engineering, Cornell University — Translational and orientational excluded volume fields can guide assembly of particles with anisotropic shape to diverse morphologies. A roadmap elucidating correlations between phase behavior and particle shape may help devising efficient strategies for self-assembly of desired nanocrystal superlattices. To explore these complex correlations we performed detailed Monte Carlo simulations of six convex multi-faceted shapes belonging to the diverse class of space-filling polyhedrons. Simulations predict formation of various novel liquid-crystalline and plastic-crystalline phases at intermediate volume fractions. By correlating these findings with particle anisotropy and order of rotational symmetry, simple guidelines for predicting phase behavior of polyhedral particles are proposed. Moreover, detailed analysis of the structures of mesophases reveals importance of dynamical order in defining these phases and preliminary information about kinetics of these transitions is also obtained. Finally, to elucidate the effect of particle shape anisotropy on rheology, preliminary results will be reported from non equilibrium molecular dynamics simulations of the isotropic and cubatic(LC) phase of cuboidal particles.

¹This work was supported by a Department of Energy Basic Energy Science Grant ER46517

11:51AM W9.00004 Triblock Janus Spheres, QIAN CHEN, SUNG CHUL BAE, STEVE GRANICK, University of Illinois at Urbana Champaign — We show that spheres that attract one another on two polar regions but repel at the middle band (“triblock Janus”) assemble into nontrivial reticulated networks. We have constructed such spheres and have visualized their aqueous assembly dynamics on the single-particle level. The building blocks are simple micron-sized colloidal spheres whose interactions (electrostatic repulsion in the middle, hydrophobic attraction at the poles) are likewise simple, but their self-assembly into this open structure contrasts with previously-known close-packed periodic arrangements of spheres. This strategy of “convergent” self-assembly from facilely fabricated colloidal building blocks encodes the target supracolloidal architecture not in localized attractive spots but rather in large redundantly attractive regions of the building blocks. The idea extends to designing other supracolloidal networks.

12:03PM W9.00005 Novel structure formation of dipolar Janus particles (JP) in electrolytes: A molecular dynamic (MD) simulation study, MAHDY MALEKZADEH, BAMIN KHOMAMI, Materials Research and Innovative Laboratory (MRAIL), Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville — There have been tremendous number of experimental studies and number of simulations in recent years trying to elucidate the underlying principals which determine structure formation of colloidal systems of JP. However most of simulations utilize relatively simple models and lack inclusion of long range columbic interactions. In this work MD simulations have been performed to understand effects of surface charge density and volume fraction (0.01-0.17) on structure formation and radial pair distribution function (RDF) of JPs of 6 nm in diameter with opposite charges on each hemisphere. Inclusion of long range columbic interaction via Ewald summation leads to formation of novel structures such as rings, chains and layered large spheres (about hundreds of nanometers) in accord to experimental observations. Moreover based on possibility of defect formation during synthesis, defects were introduced into each JP by slightly altering the uniform charge distribution on each hemisphere. Our results show in presence of small amount of defects (<10%) no significant changes occur in RDF, however increasing defect sites up to around 20% will significantly changes structure formation and combination of aforementioned structures concur to SFM and SEM images.

12:15PM W9.00006 Glassy Dynamics in the Rotator Phase of Two-Dimensional Janus Crystals, JING YAN, SHAN JIANG, JONATHAN WHITMER, STEPHEN ANTHONY, ERIK LUIJTEN, Department of Materials Science and Engineering and Department of Engineering Sciences and Applied Mathematics, Northwestern University, STEVE GRANICK, Departments of Materials Science and Engineering, Physics, and Chemistry — Janus particles, spheres with two different sides, represent the simplest building blocks whose interparticle interaction is orientation dependent. When confined on regular lattices, they epitomize basic physical problems from the arrangement of spins in magnetic materials, to rotating molecules in plastic crystals. Here we study both in experiment and in simulation, the heterogeneous dynamics in a two-dimensional crystal of amphiphilic Janus spheres. Single particle tracking reveals that orientation along can generate phenomenology resembling conventional translational supercooled liquids and glasses. Characteristic cage break events, which requires anti-correlated rotation of particles sitting on neighboring lattices, were indentified and characterized in detail. Recent experiments aiming at selectively perturbing the system using external field, such as magnetic field, will also be discussed.

12:27PM W9.00007 Chiral Control of Interfacial Tension, MARK ZAKHARY, THOMAS GIBAUD, EDWARD BARRY, ROBERT MEYER, ZVONIMIR DOGIC, Brandeis University — The interfacial tension between molecular species in self-assembling systems plays a crucial role in determining the physical properties of the mesoscopic assemblages. The predominant method for controlling interfacial tension is the addition of surfactant molecules, which preferentially adsorb onto the interface and modify the interactions between the two phases. In this talk, using a model colloidal membrane composed of chiral, rod-like *fd* viruses, I will present a new method for controlling interfacial tension which does not require additional surfactant components, but instead utilizes the intrinsic chirality of the constituent rods. I will demonstrate that chirality can be used to continuously tune the interfacial tension of a membrane and to drive a dramatic phase transition from two-dimensional membranes to one-dimensional twisted ribbons. Using a wide variety of microscopic techniques, this transition is characterized over all relevant length-scales, ranging from nanometers to microns.

12:39PM W9.00008 ABSTRACT WITHDRAWN —

12:51PM W9.00009 Dynamics of a compound vesicle in shear flow, SHRAVAN VEERAPANENI, NYU, YUAN-NAN YOUNG, NJIT, PETIA VLAHOVSKA, Brown University, JERZY BLAWZDZIEWICZ, Texas Tech University — The dynamics of compound vesicle (a lipid bilayer membrane enclosing a fluid with a suspended particle) in shear flow is investigated using both numerical simulations and theoretical analysis. We find that the non-linear coupling (via hydrodynamic interaction) between the inclusion motion and the confining membrane deformation gives rise to new features in the vesicle dynamics. Transition from tank-treading to tumbling can occur even in the absence of any viscosity mismatch. An initially non-concentric inclusion induces transient vesicle waltzing. A swinging-like vesicle motion is observed if the enclosed particle is an ellipsoid. The rheology of a suspension of compound vesicles is also strongly affected by the inclusion confinement. Our results highlight the complex effects of internal cellular structures on cell dynamics in external flow.

1:03PM W9.00010 Exploring Structure, Shape, and Dynamics of Elastin-like Polypeptide Nanoparticles, KIRIL A. STRELETZKY, Cleveland State University, KAITLIN VANDEMARK, ALI GHOORCHIAN, NOLAN HOLLAND, Cleveland State University — Environmentally responsive nanoparticles synthesized from elastin-like polypeptides (ELP) present a promising system for applications as biosensors, drug delivery vehicles, and viscosity modifiers. These nanoparticles undergo a transition from a soluble state at room temperature to micellar aggregates above the transition. The size, shape, and dynamics of micelles above the transition as well as effects of the solvent salt concentration and pH on the transition are important to understand from a fundamental science point of view as well as for potential applications. The system has been characterized with high resolution multiangle Dynamic and Static Light Scattering Spectroscopies. It was confirmed that the system undergoes a transition from mixture of ELP extended trimers and their non-spherical formations to a solution of micelles. It was discovered that micellar size and structure are very sensitive to solution's pH. The micelles were generally found to exhibit properties of the hyperbranched spheres below pH of 10 and above pH of 10.3 with their shape becoming significantly elongated in the pH window of 10 to 10.3. It was also found that the size of micelles strongly depends on salt concentration displaying at least two size regimes (20-45nm at 0-20mM and 100-150nm at 25-40mM) with different salt concentration dependences.

1:15PM W9.00011 The Lipid domain Phase diagram in a Dipalmitoyl-PC/Docosahaexnoic Acid-PE/Cholesterol System¹, CHAI LOR, LINDA HIRST², University of California, Merced — Lipid domains in bilayer membrane and polyunsaturated fatty acids (PUFAs) are thought to play an important role in cellular activities. In particular, lipids containing docosahaexnoic acid are an interesting class of PUFAs due to their health benefits. In this project, we perform oxidation measurements of DHA-PE to determine the rate of oxidation in combination with antioxidants. A ternary diagram of DPPC/DHA-PE/cholesterol is mapped out to identify phase separation phenomena using atomic force microscope (AFM). Fluorescence microscopy is also used to image lipid domains in a flat bilayer with fluorescent labels. As expected, we observe the phase, shape, and size of lipid domains changes with varying composition. Moreover, we find that the roughness of the domains changes possibly due to overpacking of cholesterol in domains. This model study provides further understanding of the role of cholesterol in the bilayer membrane leading towards a better understanding of cell membranes.

¹NSF award # DMR 0852791, "CAREER: Self-Assembly of Polyunsaturated Lipids and Cholesterol In The Cell Membrane."

²Ph.D

1:27PM W9.00012 Interfacial Microrheology with a Magnetic Needle Viscometer and Two-Particle Correlated Motion, JAMES SEBEL, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — We measure the viscoelastic moduli of thin films using two different methods. First, we use a magnetic needle viscometer. Our apparatus employs Helmholtz coils to control the position and orientation of the needle in the film. By driving the needle we can produce a response in the film which allows us to probe the bulk viscoelastic properties of the film. Second, we use two particle microrheology to probe the local properties of the film. Tracking the correlated motion between two particles as they undergo Brownian motion probes the local viscoelastic properties of any heterogeneous domains. Examining the correlations between pairs of particles with large separations helps us infer information about the bulk properties. Coupling this technique with the magnetic needle viscometer provides information on the effect local viscoelastic properties have on the bulk properties.

1:39PM W9.00013 Ion-Specific Induced Charges at Aqueous Soft Interfaces¹, WENJIE WANG, ALEX TRAVESSET, DAVID VAKNIN, Ames Laboratory, and Department of Physics, Iowa State University, Ames, Iowa 50011 — Surface-sensitive X-ray scattering and spectroscopic techniques are employed to monitor ion binding specifically to Langmuir monolayers of densely packed carboxyl or phosphate groups. By systematically varying pH of Fe³⁺, Fe²⁺ and La³⁺ solutions, we show that the critical surface pressure at the tilted (L2) to untilted (LS) transition is ionic specific and pH dependent. While the maximum density of surface bound La³⁺ per carboxylic group is ~ 0.3, the amount necessary to neutralize the fully charged surface, for Fe³⁺ it is nearly 0.6. Furthermore, the binding of Fe³⁺ is accompanied with a significant accumulation of Cl⁻ co-ions implying interfacial charge inversion. Similar experiments with charged phosphate groups at the interface show that the bindings of Fe²⁺ and La³⁺ are electrostatically driven. Our results have implications on biomineralization processes and ionic functions at cell membranes.

¹Supported by the Office of BES, U.S. Department of Energy Cont. No. DE-AC02-07CH11358.

1:51PM W9.00014 Structural characterization of a multiple stacked supported bilayer system, CURT DECARO, JUSTIN BERRY, LAURENCE LURIO, Northern Illinois University, YICONG MA, GANG CHEN, SUNIL SINHA, University of California San Diego, LOBAT TAYEBI, ATUL PARIKH, University of California Davis — Supported Lipid Bilayers are a popular model system for cell membranes since their defined orientation allow characterization with probes such as AFM, x-ray and neutron scattering. A significant concern, however, is that strong interactions with the substrate can suppress dynamics within the bilayer. One method that has been successful at overcoming this limitation is to cushion the supported bilayer on a softer material. In the present work, we have stacked up to five successive bilayers of DPPE on top of each other, in effect using the lower bilayers as cushions. X-ray reflectivity shows that each stack preserves the orientation of the first, and that each bilayer exhibits full coverage of the one below. The roughness of each bilayer is found to increase with distance from the substrate as would be expected if thermal fluctuations are increasing with distance from the substrate. We also find that upon heating from the gel to the fluid state that an unbinding transition is observed.

2:03PM W9.00015 Shape and Size of highly concentrated micelles in CTAB/NaSal solutions by small angle neutron scattering (SANS), HU CAO, HELMUT KAISER, NARAYAN DAS, PAUL SOKOL, Center for the Exploration of Energy and Matter, Indiana University, Bloomington, IN 47408, JOSEPH GLADDEN, Dept. of Physics and Astronomy, University of Mississippi, University, MS 38677 — Highly concentrated micelles CTAB/NaSal with a fixed salt/surfactant ratio of 0.6 have been studied by small angle neutron scattering (SANS) as a function of temperature and concentrations. A modeling analysis with a combination of ellipsoid, Gaussian size distribution and Hard Sphere Model (HSM) on SANS data suggests that these micelle solutions have an ellipsoidal structure, which is independent on the concentrations and temperature. However, the micelle size decreases monotonically as increasing the temperature or concentration. Besides, it was found that the number density of particles increases as increasing the temperature, while the total volume keeps unchanged. These observations indicate that large micelles at low temperature begin to break to form small ones as increasing the temperature and these broken surfactant molecules aggregate again under the effect of strongly binding counterions to form more micelles.

Thursday, March 24, 2011 2:30PM - 5:54PM –
Session X9 DFD: Coordination, Coherence and Synchronization through Hydrodynamic Interactions D220

2:30PM X9.00001 Collective motion and density fluctuations in swimming bacteria, HEPENG ZHANG, University of Texas at Austin and Shanghai Jiao Tong University — The emergence of collective motion such as in fish schools, mammal herds, and insect swarms is a ubiquitous self-organization phenomenon. Such collective behavior plays an important role in a range of problems, such as spreading of diseases in animal or fish groups. Current models have provided a qualitative understanding of collective motion, but progress in quantitative modeling is hindered by the lack of experimental data. Here we examine a model microscopic system, where we are able to measure simultaneously the positions, velocities, and orientations of up to a thousand bacteria in a colony. The motile bacteria form closely-packed dynamic clusters within which they move cooperatively. The number of bacteria in a cluster exhibits a power-law distribution truncated by an exponential tail, and the probability of finding large clusters grows markedly as bacterial density increases. Mobile clusters cause anomalous fluctuations in bacterial density as found in mathematical theories and numerical models. Our results demonstrate that bacteria are an excellent system to study general phenomena of collective motion.

3:06PM X9.00002 Collective behavior of spinning particles at fluid/fluid interface¹, YAOUEN FILY, Syracuse University, APARNA BASKARAN, Brandeis University, M. CRISTINA MARCHETTI, Syracuse Biomaterials Institute and Syracuse University — Rotating particles in a viscous fluid can exhibit interesting behavior due to hydrodynamic interactions. When the particles are driven by an external torque, these interactions result in an effective azimuthal force, leading to swirling motion. It has been shown that small numbers of such particles form precessing atom-like structures. The behavior of large collections of spinning particles is, however, still relatively unexplored. We study the phase diagram of a collection of spinning particles in two dimensions using molecular dynamics simulations. The rotors interact via hydrodynamic interactions and short-range repulsion, in the presence of thermal noise. The repulsive interaction yields transitions from a solid to a liquid to a gas as the density of rotors is decreased. The azimuthal hydrodynamic interaction modifies each of these phases in a distinct way. Both long-range and screened hydrodynamic interactions are considered. Some properties of the various phases are shown to depend critically on the range of the interaction.

¹Supported by the NSF through grants DMR-0806511 and DMR-1004789.

3:18PM X9.00003 ABSTRACT WITHDRAWN –

3:30PM X9.00004 Synchronization phenomena in systems with magnetodipolar interactions, ANDREJS CEBERS, MIHAILS BELOVS, University of Latvia — Rich pattern formation phenomena under the action of AC field for two dimensional systems of magnetic dipoles floating on the surface of liquid are observed and reproduced numerically by the first-principles model [1]. Here by the study of dynamics of two dipoles interacting with weak dipolar forces it is found that due to series of bifurcations the motion of dipoles in AC field is synchronized. If the dipoles orientation is confined to the plane the synchronous oscillation regime by infinite period bifurcation transforms to the regime of synchronous rotation. This regime is unstable for intermediate values of the field strength and the motion of dipoles is periodic or quasi-periodic. Above the critical value of field strength these regimes transform to rotational regime and the dipoles synchronously rotate in plane. Estimate of the critical parameters of the synchronization according to the dimensionless parameters used in the first-principles model [1] show that the synchronization of the dipoles rotation should be inherent in this model.

[1] M.Belkin, A.Glatz, A.Snezhko, and I.S.Aranson, Phys.Rev.E, 82, 051301(R), (2010)

3:42PM X9.00005 Pattern Formation in a Rotating Suspension of Non-Brownian Buoyant Particles, PINGER TONG¹, Department of Physics, Hong Kong University of Science and Technology, MAKRAND KALYANKAR, BRUCE ACKERSON, Department of Physics, Oklahoma State University, W.R. MATSON, Department of Physics, DePaul University — This study examines concentration and velocity patterns observed in a horizontal rotating cylinder completely filled with a monodisperse suspension of non-Brownian buoyant particles. The unique patterns or phases are mapped by varying both the rotation rate and the solvent viscosity. Individual phases are identified using both frontal and axial views. Phase boundaries are compared to those obtained recently for suspensions of non-buoyant particles. Expressing the boundaries in terms of dimensionless parameters unifies the data for several samples at low rotation rates. When centrifugal force dominates, the behavior becomes quite different from previous studies.

¹Work supported in part by the Research Grants Council of Hong Kong SAR.

3:54PM X9.00006 Shear-induced hydrodynamic diffusion of a flowing suspension of elastic capsules, MARCUS HWAI YIK TAN, DUC VINH LE, KENG-HWEE CHIAM, Mechanobiology Institute, National University of Singapore and A*STAR Institute of High Performance Computing — In flowing suspensions of soft and deformable elastic capsules, the shear flow causes hydrodynamic interaction among the capsules, resulting in an effective hydrodynamic diffusion that is not Brownian in origin. Recent experiments have suggested that hydrodynamic diffusion of red blood cells may play an important role in the pathophysiological processes of vasoocclusion and thrombosis. To study hydrodynamic diffusion further, we have developed accurate three-dimensional numerical simulations based on the immersed boundary method and thin shell theory to study the deformation of a large number of elastic capsules enclosed by thin shells moving in a shear flow. Using these simulations, we have calculated the effective hydrodynamic diffusion coefficient and showed how it varies with bulk flow velocity and capsule properties such as the volume fraction, size, and stiffness of spherical and biconcave capsules. We also compared them to scaling arguments and experimental measurements done for red blood cell suspensions.

4:06PM X9.00007 Artificial Microfluidic Squirmers, SHASHI THUTUPALLI, M.P.I. for Dynamics and Self Organisation, Gottingen, Germany, RALF SEEMANN, Physics Faculty, University of Saarlandes, Saarbrücken, Germany, STEPHAN HERMINGHAUS, M.P.I. for Dynamics and Self Organisation, Gottingen, Germany — While there is a growing consensus on the propulsion mechanisms of swimmers at low Reynolds' numbers, many questions remain open regarding the hydrodynamic effects on such swimmers, in particular the coupling between swimmers. Here we present experiments on artificial swimmers, where hydrodynamics is seen to be responsible for a wide range of collective behavior and interactions. Using droplet microfluidics with a surfactant laden continuous oil phase, we create monodisperse aqueous droplets containing chemicals that produce a steady source of Bromine ions. The surfactant (mono-olein) reacts at the droplet interface with the Bromine produced within the droplets, and a dynamic instability leads to gradients of interfacial tension at the droplet interface. These gradients set up Marangoni flows propelling the droplets, in a manner similar to the classical squirmer model of swimming. The flow around the swimmers as well as its effect on the droplet motion are measured using particle image velocimetry (PIV). The PIV analysis reveals the far field flows generated by the swimmers in the surrounding liquid, leading to the emergence of bound states and oriented clusters. We discuss the interaction mechanisms and compare it to previous theoretical work and simulations.

4:18PM X9.00008 Characterizing particle transport due to actuated cilia with adhesive tips, AMITABH BHATTACHARYA, Department of Chemical Engineering, University of Pittsburgh, GAVIN BUXTON, Department of Science, Robert Morris University, ALEXANDER ALEXEEV, Department of Mechanical Engineering, Georgia Institute of Technology, O. BERK USTA, Harvard Medical School, ANNA C. BALAZS, Department of Chemical Engineering, University of Pittsburgh — Biological tissues and organisms commonly utilize arrays of cilia to manipulate microparticles of different sizes. Motivated by biology, we use numerical simulations to study the interaction of microparticles with an array of actuated cilia, immersed in fluidic microchannel. For each cilium in the array, one end is tethered to the wall, while the other end is actuated by an external periodic force. Also, an adhesive force is introduced between the cilia tip and the microparticle. The simulations are performed using the Lattice Boltzmann Method for the flow, with a chain of point-forces, connected by springs, used to represent each cilium. We observe that a combination of hydrodynamic and adhesive forces can lead to size-specific control of microparticle transport. For instance, for certain adhesion strength and particle sizes, it is possible to trap and release particles by varying the actuation frequency. Also, for a given actuation frequency, the average particle speed is maximized at a particular adhesion strength. We will present the parameter range where we can observe the above behavior.

4:30PM X9.00009 Harnessing self-oscillating polymer gels to design active ciliated surfaces, PRATYUSH DAYAL, AMITABH BHATTACHARYA, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh — Via theory and simulations, we design active surfaces capable of replicating characteristics of biological cilia. Our approach harnesses the use of polymer gels that undergo photosensitive Belousov-Zhabotinsky (BZ) reaction. Powered by internalized BZ reaction these polymer gels swell and de-swell autonomously due to the chemo-mechanical transduction and therefore are ideal materials for designing our system. We have successfully developed an efficient hybrid approach by combining our three dimensional gel lattice spring model (3D-gLSM) and Lattice Boltzmann Method (LBM) which allows us to capture the interactions between the cilia and the surrounding fluid. Using our gLSM-LBM hybrid model we determine the factors that govern the bending and beating of individual cilium and also their collective dynamic behavior. Our findings provide guidelines for designing ciliated surfaces that can exhibit biomimetic functionality.

4:42PM X9.00010 Designing active ciliary sensors, YI YANG, ALEXANDER ALEXEEV, Georgia Institute of Technology — We employ a hybrid lattice Boltzmann / lattice spring computational model to simulate the three-dimensional hydrodynamic interactions among actuated and sensory elastic cilia tethered to a wall of a microfluidic channel. These actuated and sensory cilia are arranged a chessboard pattern on the channel wall. The actuated cilia are driven by a sinusoidal force applied to their free ends and induce periodic oscillations of a viscous fluid filling the microchannel. The passive, sensory cilia are used to measure the force arising due to fluid oscillations. We show that the combination of sensory and actuated cilia allows us to evaluate distances to solid objects located in a fluid-filled microchannel, thereby yielding a useful active sensor for microfluidic and biomedical applications.

4:54PM X9.00011 Nonlinear dynamics of flagellar bundling, PIETER JANSSEN, MICHAEL GRAHAM, University of Wisconsin - Madison — Flagella are long thin appendages of microscopic organisms used for propulsion in low-Reynolds environments. In many bacterial species, helical-shaped flagella driven by a molecular motor will bundle up. This bundling process is poorly understood, and the exact roles of hydrodynamic interactions, helix elasticity, and mechanical contact are unclear. To investigate the bundling, we consider two flexible helices next to each other, as well as several flagella attached to a spherical body. Each helix is modeled as several prolate spheroids connected by springs. For HI, we consider the flagella to be made up of point forces, while the finite size of the body is incorporated via Faxén's laws. Before flagella can bundle, they must synchronize. Synchronization occurs fast relative to the bundling process. For flagella next to each other, the initial stage of bundling is governed by rotlet interactions generated by the rotating helices. At longer times, once bundling has occurred, we find that a sharp distinction can be made between "tight" and "loose" bundles, indicated by the local distance between the flagella. As function of the anchor point distance, a sharp transition from tight to loose is found when starting from the completely unbundled state. Incremental steps from stationary situations give multiple stationary for a single anchor distance. We show that the balance between elasticity and strong non-linear hydrodynamic interactions is responsible for this bifurcation behavior.

5:06PM X9.00012 Spontaneous transitions in the synchronisation states of a *Chlamydomonas* mutant, KIRSTY WAN, KYRIACOS LEPTOS, MARCO POLIN, University of Cambridge, IDAN TUVAL, IMEDEA, Mallorca, Spain, RAYMOND GOLDSTEIN, University of Cambridge — The mechanisms by which eukaryotic flagella are found to synchronise is poorly understood; the origins being dependent upon the hydrodynamics, as well as the underlying molecular biochemistry. Exemplifying how available phenotypic variations in a species may be exploited to extend our mathematical models for flagellar coupling, we turn to ptx1 - a non-phototactic mutant strain of the biflagellated alga *Chlamydomonas* with seemingly intact flagellar apparatus, which does not exhibit any gross motility defects. Intriguingly however, our high-speed imaging analysis of flagellar dynamics in ptx1 have revealed that rather unlike their wildtype predecessors, which beat mostly in synchrony interrupted by brief periods of drifts or slip [1], the two flagella of ptx1 are observed to consistently revert from synchrony to a state of stable, coupled, anti-phase beating dynamics. Incorporating the interpretation of the flagella pair as coupled noisy oscillators, we show how such behaviour corroborates readily with a secondary contribution to the coupling, which is further conjectured to be inherent in the wildtype.
[1] Polin M et al. *Science*, 487-490, 2009.

5:18PM X9.00013 Emergence of synchronisation in flagella of variable length¹, MARCO POLIN, DAMTP, University of Cambridge, IDAN TUVAL, IMEDEA, Mallorca, Spain, RAYMOND GOLDSTEIN, DAMTP, University of Cambridge — *Chlamydomonas reinhardtii* is a unicellular green alga that can swim by the concerted breaststroke-like beating of its two flagella. When the flagella are synchronised the organism moves along a straight helical path, while a large difference in the two beating frequencies induces sharp turns. Even in the synchronous state, however, the two flagella have slightly different intrinsic frequencies, and synchrony is guaranteed only by the presence of a sufficiently strong interflagellar coupling. Although the magnitude of this coupling is consistent with the value derived from a rough hydrodynamic estimate, no direct experimental test for the role of hydrodynamic in interflagellar coupling is available. In order to better understand the origin of interflagellar coupling, we employ high-speed imaging to study the dynamics of the two flagella of *Chlamydomonas* as they regrow after mechanically induced deflagellation. Our results show that the duration of synchronised motion is strongly dependent on flagellar length. We discuss this dependence in light of hydrodynamic models of flagellar synchronisation.

¹MP acknowledges the support of the EPSRC.

5:30PM X9.00014 Fluid dynamics and noise in bacterial scattering, JORN DUNKEL, KNUT DRESCHER, University of Cambridge, LUIS CISNEROS, University of Arizona, SUJOY GANGULY, RAYMOND GOLDSTEIN, University of Cambridge — Bacterial communication through chemical and physical channels is permanently challenged by internal and external noise. While the role of stochastic fluctuations in quorum sensing has been widely studied both theoretically and experimentally, our understanding of hydrodynamic interactions between bacteria is limited by the absence of empirical data. Here, we report the first direct measurement of the fluid flow generated by an individual bacterium far away from and near to a wall. The experiments show that the micro-hydrodynamics of *E. coli* are considerably different from that of more complex eucaryotes as, for example, *Chlamydomonas* algae. We discuss the implications of our results for bacterial cell-cell and cell-wall interactions.

5:42PM X9.00015 ABSTRACT WITHDRAWN —

Thursday, March 24, 2011 2:30PM - 5:42PM —

Session X44 DPOLY DFD: Focus Session: Polymer Colloids-Structure, Function, and Dynamics

II A309

2:30PM X44.00001 Nanoparticle Organic Hybrid Suspensions: Structure and Rheology, SAMANVAYA SRIVASTAVA, LYNDEN ARCHER, Cornell University — Nanoparticle Organic Hybrid Materials (NOHMs) are a new class of tethered nanoparticle systems with high grafting densities and behave as model systems for studying spherical polymer brushes. Here we report rheology and scattering measurements of NOHMs with a silica core and PEG corona suspended in PEG oligomers at varying volume fractions. Our rheology results reveal a liquid-glassy transition at strikingly low core volume fractions in these suspensions and prominent stress overshoots in flow startups indicative of yielding in the high volume fraction suspensions. Further, we elucidate the form of particle interactions in the glassy suspensions and compare them with established models. Also, a negative first normal stress difference in the moderate volume fraction suspensions is reported, which is in agreement with recent theoretical and experimental findings. We also report small angle scattering measurements of these suspensions to reveal their equilibrium structure, which are in qualitative agreement with a recent theoretical study (Langmuir, 2010, 26, 16801).

2:42PM X44.00002 Measuring and Modeling the Interactions Between DNA-Functionalized Colloids, WILLIAM ROGERS, JOHN CROCKER, Department of Chemical and Biomolecular Engineering, University of Pennsylvania — DNA hybridization is an ideal tool to direct “bottom-up” assembly of complex materials and has been used to form crystalline assemblies of quantum dots, polymer microspheres and other materials made exclusively of DNA. In order to fully realize the potential of DNA-directed self-assembly, one must be able to quantitatively predict the binding energies and interaction potentials between the relevant “building blocks.” In this work, we use a scanning-line optical tweezers instrument to measure DNA-induced interactions between colloidal microspheres. We then use well-known concepts in statistical mechanics to model the pair-potentials, whose functional form and energetics of binding are intimately related to the equilibrium configurations of grafted polymers and polymer bridges. By measuring and modeling the pair interaction energies as a function of the essential system parameters (solution hybridization free energies, DNA concentrations, temperature, interparticle separation, etc.), we are able to develop simple, numerical tools that can be used to guide both experiment and simulation.

2:54PM X44.00003 Rheological and scattering properties of cross-linker-free microgels, ZHIYONG MENG, CHINEDUM OSUJI, Yale University — Microgel suspensions are intriguing tunable systems in part due to their pH/temperature responsivity at the single particle level. Particle collapse during volume transitions is heavily mediated by the presence of cross-links in the system. Here we examine the rheology and light scattering of microgel suspensions based on poly(*N*-isopropylacrylamide-co-acrylic acid) (pNIPAM-AAc) in the limit of vanishing cross-linking density. One issue of concern is centered on the nature of these fluids – are they simple polymer solutions or real particulate suspensions? A combination of concentration-dependent viscometry and static light scattering demonstrates conclusively that these are particulate suspensions. The absence of cross-linkers provides a sharper volume collapse at the LCST in comparison with heavily cross-linked particles. Furthermore, at fixed mass content, cross-linker-free microgel suspensions display a much higher shear modulus than cross-linked counterparts due to their larger particle size, which implicates the use of these particles in rheological modification. We survey the frequency dependence and yielding response of these suspensions as a function of temperature and composition.

3:06PM X44.00004 Normal Modes and Density of States of Disordered Colloidal Solids, MOHAMMAD ISLAM, Department of Materials Science & Engineering, Carnegie Mellon University, Pittsburgh, PA 15213 — The normal modes and the density of states (DOS) of any material provide a basis for understanding its thermal and mechanical transport properties. In perfect crystals, normal modes take the form of planewaves, but they can be complex in disordered systems. I will show our recent experimental measurements of the normal modes, the DOS and dynamical structure factor (DSF) in disordered colloidal solids: disordered colloidal crystals composed of thermally sensitive micron-sized hydrogel particles at several different particle volume fractions, ϕ . Particle positions are tracked over long times using optical microscopy and particle tracking algorithms in a single two dimensional (2D) [111] plane of a 3D face-centered-cubic single crystal. The dynamical fluctuations are spatially heterogeneous while the lattice itself is highly ordered. At all ϕ , the DOS exhibits an excess of low frequency modes, a so-called boson peak (BP), and the DSF exhibits a crossover from propagating to non-propagating behavior, a so-called Ioffe-Regel (IR) crossover, at a common frequency somewhat below the BP for both longitudinal and transverse modes. As we tune ϕ from 0.64 to 0.56, the Lindemann parameter grows from $\sim 3\%$ to $\sim 8\%$, however, the shape of the DOS and DSF remain largely unchanged when rescaled by the Debye level. This invariance indicates that the effective degree of disorder and the structure of the underlying normal modes remain essentially unchanged even in the vicinity of melting. This work was supported by NSF through grants DMR-0645596 & DMR-0619424, the Sloan Foundation and American Chemical Society Petroleum Research Fund.

3:42PM X44.00005 Signatures of Aging: Comparison between Colloidal and Molecular Glasses, XIAOJUN DI, Dept of ChE, Texas Tech Univ., K.Z. WIN, GREGORY MCKENNA, T. NARITA, F. LEQUEUX, S. PULLELA, Z. CHENG, DEPT OF CHE, TEXAS TECH UNIV TEAM, PPM, UPMC-ESPCI-CNRS, FRANCE TEAM, DEPT OF CHE, TEXAS A&M UNIV TEAM — Colloids near to the glass concentration are often taken as models for molecular glass formers. Yet, one of the most important aspects of the dynamics of molecular glasses, structural recovery, remains to be examined in colloids. We use DWS to investigate structural recovery in a thermosensitive PNIPAM colloidal suspension in the glass concentration range. The three classical aging signatures observed in molecular glasses: intrinsic isotherms, asymmetry of approach and memory effect, are investigated with this colloid and the results are compared with those typical of molecular glasses. We find: 1 for the intrinsic isotherms, the colloid shows dramatic changes in relaxation time at equilibrium while the times required to reach the equilibrium state are nearly independent of the concentration; 2 for the asymmetry of approach, the observed nonlinearity is similar to that in molecular glasses; 3 for the memory experiment, while the memory effect is seen in the colloid, the response is qualitatively different than in the molecular glass.

3:54PM X44.00006 Packings of soft disks¹, PRIMOZ ZIHERL, University of Ljubljana and Jozef Stefan Institute, MARIJA VIDMAR, University of Ljubljana — We explore the stability of 2D ordered structures formed by soft disks treated as isotropic solid bodies. Using a variational model, we compute the equilibrium shapes and the elastic energy of disks in regular columnar, honeycomb, square, and hexagonal lattice. The results reproduce the Hertzian interaction in the regime of small deformations. The phase diagram of elastic disks is characterized by broad regions of phase coexistence; its main feature is that the coordination number of the stable phases decreases with density. These results may provide an insight into structure of the non-close-packed lattices observed in certain nanocolloidal systems.

¹This work was supported by Slovenian Research Agency (grant No. P1-0055) and by EU through ITN COMPLEIDS (grant FP7-People-ITN-2008 No. 234810).

4:06PM X44.00007 Theory of effective interactions and dispersion of soft nanoparticles in polymer melts, JIAN YANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — Integral equation theory is employed to investigate the consequences of nanoparticle softness (surface fluctuations) and corrugation (discrete roughness) on the equilibrium behavior of polymer-particle mixtures in the dilute filler limit. Monomer-particle pair correlations exhibit qualitatively different features relative to hard spheres which depend on both roughness and softness. Under athermal nonadsorbing polymer conditions, depletion effects on the interparticle potential-of-mean-force (PMF) are qualitatively modified by surface corrugation and/or fluctuations. As particle softness increases, monomer-scale PMF oscillations are destroyed, and the strongest attraction occurs at a particle separation and attraction depth that depends sensitively on surface fluctuation amplitude, as does the dependence on monomer-nanoparticle size asymmetry ratio (R). For corrugated particles, the most attractive nanoparticle separation does not occur at contact, and is far weaker and less sensitive to R than for hard spheres. Second virial coefficient calculations are performed to estimate how particle softness/roughness modifies miscibility in chemically matched blends. How surface corrugation and softness modifies bridging and sterically stabilized states has also been studied.

4:18PM X44.00008 Density functional theory for the structure and dynamics of solvent-free nanoparticle-organic hybrid materials, HSIU-YU YU, DONALD KOCH, Cornell University — Nanoparticle-organic hybrid materials consist of inorganic nanocores functionalized with oligomeric organic molecules. They exhibit fluid behavior in the absence of solvent with the fluidity provided by the attached oligomers. We present a density-functional theory for the equilibrium structure and transport properties of these materials based on an assumption that the intercore forces are mediated by entropic effects associated with the conformations of the hairs subject to the constraint that the oligomer fluid is incompressible. Because each core particle carries its share of the fluid phase, the structure factor at zero wave number is equal to zero. When the radius of gyration of the oligomers is large compared with the core radius, each core experiences weak interactions with many other cores residing in its neighborhood. Exploiting this limit, the transport properties can be determined in a quasi-analytical manner based on a solution of the non-equilibrium probability density for pairs of particles experiencing a non-pairwise-additive intercore potential.

4:30PM X44.00009 Yielding mechanisms and particle rearrangements in colloidal glasses and gels under shear, GEORGE PETEKIDIS, IESL-FORTH — Steady and oscillatory rheology was utilized to study the mechanical response of colloidal glasses and gels with particular emphasis in the way these are shear melted (yield) [1,2]. We used suspensions of hard sphere colloids with short-range depletion attractions induced by the addition of non-adsorbing linear polymer. The linear viscoelasticity and the yielding mechanisms at different regimes of colloid volume fraction and particle attractions are discussed. While hard sphere glasses exhibit a single step yielding due to cage breaking, attractive glasses show a two-step yielding reflecting bond and cage breaking respectively [1]. Here we present experimental data both along a line of equal attraction, varying the particle volume fraction, from an attractive glass to a low volume fraction gel as well as at intermediate and high volume fractions with increasing the attraction strength. In attractive gels yielding remains a two step process until very low ϕ 's. The first yield strain is related with in-cage or inter-cluster bond braking while the second yield point is attributed to braking of cages or clusters into smaller constituents [3]. The latter increases as volume fraction is decreased due to enhancement of structural inhomogeneities. When the range of attraction was increased, both yield strains increase, scaling with the range of attraction and accompanied structural changes. Brownian Dynamics simulations and Dynamic Light scattering under shear (LS-echo) provide information on the microscopic particle rearrangements and structural changes during yielding and flow such as the size and structure of clusters that change under steady shear as a function of shear rate. Work in collaboration with: N. Koumakis, (FORTH), M. Laurati, S.U. Egelhaaf (U. Duesseldorf) and J. F. Brady (Caltech).

[1] K. Pham et al. *J. Rheology* 52, 649 (2008)

[2] M. Laurati, *J. Chem. Phys.* 130, 134907 (2009)

[3] Koumakis and Petekidis, submitted (2010); Laurati et al, submitted (2010)

5:06PM X44.00010 Ridge formation of charged end group ligands grafted on faceted nanoparticle, PEIJUN GUO, RASTKO SKNEPNEK, MONICA OLVERA DE LA CRUZ, Northwestern University — We have investigated the conformations of charged end group ligands grafted on icosahedral nanoparticles, using a coarse-grained molecular dynamics approach. Due to a competition between the electrostatic repulsion and the hydrophobic ligand-ligand attraction, the ligand coatings form a variety of different conformations. These conformations have been compared with the case of non-charged grafted ligands. We have found that the electrostatic interaction between the charged ends drives the formation of a ridge-like structure of the ligands, which makes the nanoparticle surface highly anisotropic. We argue that the ridge-like ligand structure induces controllable directional interaction between the nanoparticles, and can drive the self-assembly of the nanoparticles into crystalline structures.

5:18PM X44.00011 Dynamics of Polymers in Colloidal Flows, HSIEH CHEN, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — This research is motivated by recent studies on the von Willebrand factor (vWF), a large multimeric protein that plays an essential role in the initial stages of blood clotting in blood vessels. Recent experiments substantiated the hypothesis that the vWF is activated by shear stress in blood flow that causes its shape to transform from a compact globule to an extended state [1], and biological function is obtained only in the extended state. Simple simulations (which only consider a single polymer in bulk shear flow) have successfully reproduced the observed dynamics of the vWF [2]. However, a more refined model is still demanding for the better understanding of the behaviors of this biomolecule in the physiological environments. Here we refine the existing model by adding the drifting colloids into the flows to mimic the presence of the blood cells in the bloodstream. Preliminary result shows that colloids greatly influence the dynamics of the polymers. It is observed that the average extensions of polymers along and perpendicular to the shear flow direction are both increased with the presence of the colloids.

[1] S.W. Schneider, et. al. *PNAS* (2007) 104 19 7899-7903

[2] A. Alexander-Katz, et. al. *Phys. Rev. Lett.* (2006) 97 13 138101

5:30PM X44.00012 Spontaneous asymmetry in coated spherical nanoparticles in solution and at liquid-vapor interfaces, J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories — Nanoparticles in solution are often stabilized with functional coatings to prevent aggregation. We'll present recent simulations results showing that small spherical nanoparticles produce highly asymmetric coating arrangements, when coated with simple polymer chains. These coatings are not symmetric even when extremely uniform grafting arrangements and full coverages are employed. I will also discuss the geometric properties which dictate the coating shape. When particles are placed in an anisotropic environment, such as the liquid/vapor interface, the asymmetric coatings are amplified and oriented by the surface. Particle shape and its responsive behavior is seen to strongly influence interactions. Implications and examples of controlled self-assembly will be presented.

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y9 DFD: Motility, Locomotion and Cellular Fluid Mechanics D220

8:00AM Y9.00001 ABSTRACT WITHDRAWN –

8:12AM Y9.00002 Coordinated Swimming: Hydrodynamic interactions between multi-flagellated bacteria, NOBUHIKO WATARI, RONALD LARSON, University of Michigan — Multi-flagellated bacteria, such as *Escherichia coli*, often have flagella attached at random locations to the cell body, which drive swimming behavior. To study the effect of hydrodynamic interactions on the swimming behavior, we develop a bead-spring model which represents both the body and the flagella using up to 240 Stokeslets, or hydrodynamic drag centers. These beads are bonded by 1) a spring potential, 2) a bending potential, and 3) a torsional potential to adjacent beads. This modeled bacterium swims by rotating the flagella with constant torques. We find that the number and arrangement of the flagella along the bodies of the swimmers affects how two such swimmers approach each other, when swimming either in a line, or side by side, and affects whether or not flagellar rotations are synchronized or not. We show how the flow field generated by each swimmer can be represented using a low order multipole expansion, which can capture the qualitative features of their interactions. With this simple low order expansion, simulations of hundreds or thousands of such swimmers can be carried out, allowing the effects of numbers and locations of flagella on swimming pattern formation to be captured.

8:24AM Y9.00003 Remote Powering and Steering of Self-Propelling Microdevices by Modulated Electric Field, RACHITA SHARMA, ORLIN VELEV, North Carolina State University — We have demonstrated a new class of self-propelling particles based on semiconductor diodes powered by an external uniform alternating electric field [1]. The millimeter-sized diodes floating in water rectify the applied voltage. The resulting particle-localized electroosmotic flux propels them in the direction of the cathode or the anode depending on their surface charge. These particles suggest solutions to problems facing self-propelling microdevices, and have potential for a range of additional functions. The next step in this direction is the steering of these devices. We will present a novel technique that allows on-demand steering of these self-propelling diodes. We control remotely their direction of motion by modifying the duty cycle of the applied AC field. The diodes change their direction of motion when a DC component (wave asymmetry) is introduced into the AC signal. The DC component leads to redistribution of the counterions near the diode surface. The electric field resulting from this counterion redistribution exerts a torque on the dipole across the diode, causing its rotation. Thus, the reversal of the direction of the electroosmotic flux caused by field asymmetry leads to reversal of the direction of diode motion. This new principle of steering of self-propelling diodes can find applications in MEMS and micro-robotics. [1] S. T. Chang, V. N. Paunov, D. N. Petsev, O. D. Velev, *Nat Mater*, 6, 235-240 (2007).

8:36AM Y9.00004 Motility of rotating flagella in viscoelastic fluids, BIN LIU, THOMAS POWERS, KENNETH BREUER, Brown University — Bacteria achieve motility by eluding the constraints of kinematic reversibility, for instance, by rotating a helical flagellum. We study experimentally the motility of the flagellum with a scaled-up model system, a motorized helical coil that rotates along its axial direction. The rotating helix is tethered on a linear stage that advances at a predetermined speed along the axial direction. A free-swimming speed is obtained when the net force on the helix is zero. In the Newtonian case, the free-swimming speed of the helix is always proportional to its rotation rate. We show how such motility is affected by the presence of the viscoelasticity of the fluid, a ubiquitous environment for living bacteria.

8:48AM Y9.00005 Electrical Control of Microtubule Translocation on Graphene, EUNJI KIM, Department of Biophysics and Chemical Biology, Seoul National University, Seoul 151-747, Korea, DONG SHIN CHOI, Department of Nano Science and Engineering, Seoul National University, Seoul, 151-747 Korea, KYUNG-EUN BYUN, Department of Physics and Astronomy, Seoul National University, Seoul, 151-747, Korea, HEEJUN YANG, JINSEONG HEO, HYUN-JONG CHUNG, SUNAE SEO, Semiconductor Devices Lab, Samsung Advanced Institute of Tech., Giheung-Gu, Yongin-Si, Gyeonggi-Do 449-712, Korea, SEUNGHUN HONG, Department of Biophysics and Chemical Biology, Seoul National University, Seoul 151-747, Korea — Motor protein systems such as a kinesin-microtubule complex play an important role in intracellular cargo transport by directly converting a chemical energy into a mechanical work. For exploiting their high energy efficiency, there have been considerable efforts to integrate them with various nanostructures to build nanoscale biodevices such as an advanced nano-transportation system. Herein, we demonstrated a successful motility assay of microtubules on a kinesin-functionalized graphene electrode which has a good transparency and conductivity. By applying a voltage bias onto the graphene electrode, we could spatially control the translocation of the microtubules. Our result clearly shows that graphene can be used not only as a good substrate for a motor-protein motility assay but also as a key component for a nano-mechanical system based on biomotors.

9:00AM Y9.00006 Swimming speed of an oscillating sheet in Newtonian and viscoelastic fluids, MOUMITA DASGUPTA, MICHAEL BERHANU, ARSHAD KUDROLLI, Clark University, HENRY FU, University of Nevada, Reno, KENNETH BREUER, THOMAS POWERS, Brown University — We discuss a mechanical experimental model of a flexible sheet swimming with a prescribed wave pattern - a Taylor swimmer - through a fluid. Our study is motivated by a need for a fundamental understanding of microorganism locomotion through non-Newtonian fluids. In order to simplify the problem, we suspend a tall flexible cylindrical sheet concentric within a cylindrical tank filled with the fluid. Torque free boundary conditions are imposed by supporting the flexible sheet and the tank with friction-free ball-bearings. A traveling wave is imposed on the sheet with a pair of rollers in the azimuthal direction. We first demonstrate a linear response in the swimming velocity of the sheet with respect to its phase velocity in a viscous Newtonian fluid. Further, we show that the analytical system is essentially two dimensional by varying the height of fluid in the tank. We then discuss measurements of swimming speed in Polyox-water mixtures as a function of wave speed. We demonstrate that the swimming speed in this viscoelastic fluid decrease relative to the Newtonian case as wave speed is increased. We will further discuss the dependence of swimming speed on Deborah number and other characteristics of the fluid.

9:12AM Y9.00007 Highly-Controllable Near-Surface Swimming of Magnetic Nanorods, BENJAMIN EVANS, Elon University, LAMAR MAIR, UNC - Chapel Hill — Directed manipulation of nanomaterials has significant implications in the field of nanorobotics, nanobiotechnology, microfluidics, and directed micro- and nano-object assembly. With this in mind, we present a simple, efficient method for the fabrication and controlled manipulation of rod-shaped micro-scaled swimmers in a low-Reynolds environment. We demonstrate fine spatial control of the swimmers' motion and we approach, capture, and manipulate a polystyrene microbead as proof of principle. The swimmers consist of 200-nm-diameter gold nanowires which are grown by electrodeposition in an AAO template. The template is removed via dissolution in NaOH, and a layer of nickel (50 nm) is subsequently evaporated onto the surface of the wires. These wires settle near the floor of an enclosed water-filled cell and are observed via optical microscopy. Rotation is induced via an external magnetic field provided by a permanent magnet. The field is rotated in a plane nearly parallel to the floor; a small tilt out-of-plane results in symmetry-breaking, with the end of the rod nearest the floor experiencing an enhanced drag coefficient due to the presence of the boundary. The imbalance in drag forces between the two ends of the rotating rod results in a net translation. We use resistive force theory to develop an analytical model which describes the motion of these swimmers and correlate this model with experimental results.

9:24AM Y9.00008 Textured boundaries and their effects on ciliary locomotion, SAIKAT JANA, Department of Engineering Science and Mechanics, Virginia Tech, SUNG YANG, Department of Nanosystems and Engineering, GIST, South Korea, SUNGHWAN JUNG, Department of Engineering Science and Mechanics, Virginia Tech — Many microorganisms in nature propel themselves by creating coordinated motion of the cilia and often interact with each other through hydrodynamic interactions. We study the behavior of these organisms near boundaries of different topography and rationalize the hydrodynamic effects involved. Various geometries like wavy, rough or solid walls are simulated using micro fabrication and their effects on the locomotory traits are observed. Finally a comprehensive discussion on the effect of different boundaries on the swimming characteristics of the organism is presented.

9:36AM Y9.00009 Motion of Elastic Microcapsules on Compliant Surfaces with Adhesive Ligands, EGOR MARESOV, GERMAN KOLMAKOV, ANNA BALAZS, University of Pittsburgh — By integrating mesoscale models for hydrodynamics, micro-mechanics and adhesion, we examine the fluid driven motion of elastic microcapsules on compliant surfaces. The capsules, modeled as three-dimensional fluid-filled elastic shells, represent polymeric microcapsules or biological cells. Our combined integrated Lattice Boltzmann model/Lattice spring model (LBM/LSM) approach allows for a dynamic interaction between the elastic capsule's wall and surrounding fluid. To capture the interaction between the shell and the surface, we adopt the Bell model, used previously to describe the interaction of biological cell like leukocytes rolling on surfaces under the influence of an imposed shear. The surface of the microcapsule contains receptors with an affinity to adhesive ligands of the substrate. We examine how the parameters of adhesion and rigidity of the capsules and the substrate affect movement of the capsules. The findings provide guidelines for creating smart surfaces that could regulate the microcapsules' motion.

9:48AM Y9.00010 Modelling the dynamics of colloidal nanorods in a spatially varying electric field, GREGORY RICHARDS, Dept. of Mathematical Sciences and Liquid Crystal Institute - KSU, XIAOYU ZHENG, Dept. of Mathematical Science - KSU, PETER PALFFY-MUHORAY, Liquid Crystal Institute - KSU — The behavior of anisotropic nanoparticles is of great current interest in the design of optical metamaterials. We have carried out numerical simulations to model the dynamical behavior of metallic nanorods, dispersed in an isotropic solvent, under the influence of a radially varying electric field. Diffusive and convective transport is considered both in orientation and position space. The Smoluchowski equation governing the spatial and orientational probability density function (PDF) was derived. Discretization was carried out using a finite-volume method on a mesh generated via Voronoi tessellation and regularization on the unit sphere. The time evolution of the PDF was obtained using a combination of operator splitting and a stable biconjugate gradient method. We present the results of our numerical experiments. We report interesting and anomalous behavior, where, due to the coupling of orientation and translational mobility, the applied field depopulates certain orientational states, similar to 'orientational hole burning' in nonlinear optics.

10:00AM Y9.00011 Designing self-propelling micro-swimmer that navigates in microfluidic channels, BEN BINGHAM, HASSAN MASOUD, ALEXANDER ALEXEEV, Georgia Institute of Technology — Using a fully-coupled computational approach that integrates the lattice Boltzmann model for the hydrodynamics and the lattice spring model for the micromechanics of deformable solids, we design a synthetic micro-swimmer that not only self-propels but also successfully navigates in a low Reynolds number environment of a microfluidic channel. The swimmer body consists of a responsive polymer gel that undergoes periodical swelling and shrinking. Two thin elastic flappers are attached to the opposite sides of the swimmer body. The flappers wiggle driven by swimmer body oscillations and, in this fashion, propel the micro-swimmer through its highly viscous fluid environment. Third, light sensitive flapper is attached in the front of the swimmer and serves to steer its trajectory in microchannel. When exposed to light, the steering flap bends towards the light source. We show that this swimmer can either move straight or turn in the required direction following light signals. Thus, guided by light, the micro-swimmer can successfully navigate towards the target in a microfluidic channel.

10:12AM Y9.00012 Azobenzene Crystal Shooting and Shape Behavior in the Context of Time Dependent Ginzburg-Landau Equations¹, THOMAS SUTTER, Polymer Engineering, University of Akron, GRANG RILEY, Physics Department, Miami University, DMITRY GOLOVATY, Theoretical and Applied Mathematics, University of Akron, THEIN KYU, Polymer Engineering, University of Akron — Blends of azobenzene chromophore and diacrylate monomer show novel nucleation instability. Once a crystal nucleates near a larger growing crystal, it shoots away from the growing front. This shooting phenomenon is explained in the context of "Marangoni propulsion," an imbalance of surface energies at the leading and trailing crystal edges. A concentration gradient is established during the course of diffusion-controlled crystal growth; as the crystal front pulls azobenzene molecules in and rejects acrylate solvent molecules. Thus, crystal growth dynamics influence the concentration gradient build up at the advancing front, as well as the crystal's shape. The time dependent Ginzburg-Landau model C equation was used to simulate crystal growth using a free energy expression which combines Flory-Huggins theory of liquid-liquid demixing and the phase field free energy of crystallization. We have also established a theoretical phase diagram by self-consistently solving the free energy expression. Crystal shape and shooting character will be explained in the context of the phase diagram.

¹We thank the donors of the American Chemical Society Petroleum Research Fund (PRF#48735-ND7).

10:24AM Y9.00013 Flagellar generated flow mediates attachment of *Giardia lamblia*¹, JEFFREY URBACH, HAIBEI LUO, THEODORE PICOÛ, RYAN MCALLISTER, HEIDI ELMENDORF, Georgetown University — *Giardia lamblia* is a protozoan parasite responsible for widespread diarrheal disease in humans and animals worldwide. Attachment to the host intestinal mucosa and resistance to peristalsis is necessary for establishing infection, but the physical basis for this attachment is poorly understood. We report results from TIRF and confocal fluorescence microscopy that demonstrate that the regular beating of the posterior flagella generate a flow through the ventral disk, a suction-cup shaped structure that is against the substrate during attachment. Finite element simulations are used to compare the negative pressure generated by the flow to the measured attachment force and the expected performance of the flagellar pump.

¹NIH grant 1R21AI062934-0

10:36AM Y9.00014 Probing the directional structure and intracellular microrheology of vascular endothelial cells, MANUEL GOMEZ-GONZALEZ, KATHRYN OSTERDAY, JULIE LI, GERARD NORWICH, JUAN LASHERAS, SHU CHIEN, JUAN CARLOS DEL ALAMO, University of California, San Diego — The magnitude of the rheological properties of cytoplasm is important because it sets the level of intracellular deformation in response to stress. The directionality is equally important because it allows the cell to modulate the stress-strain relation differently along different directions. We aim to elucidate the relation between the structural organization of the cytoplasm and the directionality of its rheological properties by 1) measuring the local orientation of fluorescently labeled intracellular filaments and 2) determining the local directions of the maximum and minimum intracellular viscosity. For this purpose, we improved current microrheology measurements by studying the drag force experienced by a microsphere in an anisotropic viscoelastic network permeated by a liquid. In the limit of strong frictional coupling between network and liquid, the flow around the sphere is modeled with a generalized Stokes equation using several viscosity parameters. We solve this equation analytically to provide new closed-form microrheology formulae relating the resistance measured experimentally to the anisotropic properties of the network. Tracking the random motion of endogenous particles in 2D and using these novel microrheology formulae we measured directional intracellular viscosities.

10:48AM Y9.00015 Non-equilibrium fluctuations of cell membranes: The effect of cytoskeletal motor activity on membrane dynamics, ROIE SHLOMOVITZ, ALEX LEVINE, UCLA, Department of Chemistry & Biochemistry — The mechanics and non-equilibrium (i.e. molecular motor-driven) fluctuation spectrum of living cells remains an open problem. In this talk, we explore the question: What can one infer about the action of endogenous motors in the cytoskeleton by observing the height fluctuations of cell membrane? To address this, we treat the cytoskeleton as a uniform elastic half-space bounded by a membrane with a finite bending modulus and driven out of equilibrium by molecular motors (i.e. myosin). These motors produce transient and stochastic contractile stresses in the elastic bulk. We first calculate the induced undulations of the membrane-bound surface due to the action of a single molecular motor. Then, making assumptions about the spectrum of motor force fluctuations, we calculate the expected non-thermal contribution to the cellular membrane fluctuations due to the action of an ensemble of such motors. We discuss extensions of this simple model to include, e.g. the effect spatially inhomogeneous coupling between the cytoskeleton and the membrane. We also mention ongoing experimental tests of these ideas.

Friday, March 25, 2011 8:00AM - 11:00AM –
Session Y13 GSNP DFD: Granular Materials I D225/226

8:00AM Y13.00001 ABSTRACT WITHDRAWN –

8:12AM Y13.00002 Homogeneous linear shear of a two dimensional granular system, JOSHUA A. DIJKSMAN, JIE REN, ROBERT P. BEHRINGER, Duke University — Using a novel shear device, we experimentally study the response of dry granular materials to quasi-static shear. Our apparatus is capable of creating linear strain profiles over the entire width of the two dimensional shear cell. By eliminating the usual tendency of granular shear to localize in non-uniform shear bands, we can study the poorly understood nature of granular flows in great detail. We employ photo elastic particles, fluorescent labelling and high resolution imaging to obtain information about particle positions, rotation and inter particle forces. We discuss our results in the context of the jamming scenario and also look at various measures capable of elucidating the physics of dense granular flows.

8:24AM Y13.00003 Constitutive relations for granular fluid of smooth inelastic hard spheres, to Burnett order, VINAY GUPTA, MEHEBOOB ALAM, JNCASR, Bangalore, India — In the framework of kinetic theory for dilute granular gases, we have generalized the work of Sela & Goldhirsch (1998) by including body force (gravity) term in the Boltzmann equation. In order to derive the constitutive relations for flows of smooth inelastic hard spheres in three dimensions, the Boltzmann equation is perturbatively solved by performing generalized Chapman-Enskog (double expansion) in two small parameters, the Knudsen number and the degree of inelasticity. We have derived the constitutive relations till Burnett order (up to second order in small parameters). In this talk I would like to present the methodology for obtaining the constitutive relations.

Ref: Sela, N. & Goldhirsch, I. 1998 Hydrodynamic equations for rapid flows of smooth inelastic spheres, to Burnett order. *J. Fluid Mech.* **361**, 41–74.

8:36AM Y13.00004 Random to ordered granular sphere packings through cyclic shear, ANDREEA PANAITESCU, ANKI REDDY, ARSHAD KUDROLLI, Clark University — We investigate the structure of a dense granular packing submitted to quasi-static cyclic shear deformations using a fluorescent liquid refractive index matching method. This technique allows us to obtain the three dimensional position of 1mm glass spheres in the bulk during each cycle. The granular packing is observed to evolve towards crystallization over hundreds of thousands of shear cycles and the packing fraction is correspondingly observed to increase from loose packing fraction, 0.59, to above random close packing, 0.634. The appearance and the propagation of the crystalline order was studied using the orientational order metric, Q_6 . In the early stages of nucleation the particles belonging to the nucleating crystallites are predominantly in hexagonal close packed configuration. When the packing volume fraction approaches a value close to random close packing, a rapid increase of the global Q_6 and the number of particles with local face centered cubic order is observed. Following the evolution of the crystallites, we find the critical nuclei size to be between 10-50 particles, surprisingly consistent with transitions observed with thermal elastic frictionless spheres. A detailed description of the crystalline clusters and their development will be presented.

8:48AM Y13.00005 Shearbanding Instability and Patterns in Granular Shear Flows, PRIYANKA SHUKLA, MEHEBOOB ALAM, J.N.Centre for Advanced Scientific Research, Bangalore — When a (dense) granular material is sheared in shear-cell experiments, shearing remains confined to a narrow localized zone ("shearband") near the moving boundary. Such shear-banding has also been realized in the molecular dynamics simulations of granular plane Couette flow for a range of densities (even without gravity) in the rapid flow regime. In this talk I will present the shear-banding instability of granular shear flow via an order parameter equation.

[1] Weakly nonlinear theory of shear-banding instability in granular plane Couette flow: analytical solution, comparison with numerics and bifurcation, Priyanka Shukla and Meheboob Alam, *Journal of Fluid Mechanics* 2010, **665**, p. 1-50.

[2] Landau-type order parameter equation for shear banding in granular Couette flow, Priyanka Shukla and Meheboob Alam, *Physical Review Letters*, **103**, 068001, 2009.

[3] Universality of shear-banding instability and crystallization in sheared granular fluid, Meheboob Alam, Priyanka Shukla and Stefan Luding, *Journal of Fluid Mechanics*, **615**, p. 293-321, 2008.

9:00AM Y13.00006 Shearing granular media: from elasticity to compaction, JEAN-FRANCOIS METAYER, MPI for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen, ELIE WANDERSMAN, MARTIN VAN HECKE, University of Leiden, MATTHIAS SCHRÖTER, MPI for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen — A granular system is able to behave like a solid (a sand pile for example) or like a liquid depending on the deformation imposed on the material. Using rheometry measurements we investigate the response of a granular bed to an imposed deformation or an imposed stress as a function of its packing fraction. We observed different regimes: elastic and plastic behaviors, flow regime and finally compaction. The dependence of these regimes on the packing fraction and on the pressure allows us to delineate the phase diagram of granular media.

9:12AM Y13.00007 Microscopic rearrangements and macroscopic stress fluctuations in dense emulsion flow, DANDAN CHEN, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — One characteristic of dense granular materials is they can resist small stresses but start to flow under large stresses. During granular flow, the stress exerted on the boundaries of the flow can have large fluctuations. These fluctuations are thought to originate from internal rearrangements and from changes of force chains; however, the connection between these internal microscopic changes and the macroscopic influences seen at the boundaries is not yet clear. We experimentally study the shear flow of oil-in-water emulsion droplets in a Hele-Shaw cell with a hopper shape. Due to the thinness of the Hele-Shaw cell, the droplets are deformed into quasi-2D pancakes, somewhat analogous to soft photoelastic disks. As droplets approach the hopper exit, they shear past one another and droplets are forced to rearrange. We focus on a typical plastic rearrangement called T1 event, where local four particles have neighbor exchanges. Simultaneously, we use the deformation of the droplets to determine the interdroplet forces, which also change as the sample is sheared. These forces fluctuate over large regions as expected. Our analysis of this emulsion system shows a direct and local relationship between microscopic T1 rearrangements and macroscopic stress fluctuations.

9:24AM Y13.00008 Flow and Sedimentation of particulate suspensions in Fractures¹, TAK SHING LO, JOEL KOPLIK, Levich Institute and Department of Physics, City College of CUNY — Suspended particles are commonly found in reservoir fluids. They alter the rheology of the flowing liquids and may obstruct transport by narrowing flow channels due to gravitational sedimentation. An understanding of the dynamics of particle transport and deposition is, therefore, important to many geological, environmental and industrial processes. Realistic geological fractures usually have irregular surfaces with self-affine structures, and the surface roughness plays a crucial role in the flow and sedimentation processes. Recently, we have used the lattice Boltzmann method to study the combined effects of sedimentation and transport of particles suspended in a Newtonian fluid in a pressure-driven flow in self-affine channels, which is especially relevant to clogging phenomena where sediments may block fluid flows in narrow constrictions of the channels. The lattice Boltzmann method is flexible and particularly suitable for handling irregular geometry. Our work covers a broad range in Reynolds and buoyancy numbers, and in particle concentrations. In this talk, we focus on the transitions between the “jammed” and the “flow” states in fractures, and on the effects of nonuniform particle size distributions.

¹Work supported by DOE and NERSC.

9:36AM Y13.00009 Dilation of Granular Packings of Spheres and Non-Spherical Particles under Shear, ABIGAIL POLIN, BEZ LADERMAN, CHRISTOPHER PEEL, JOHN R. ROYER, PAUL M. CHAIKIN, New York University — A parallelepiped shear cell is used to experimentally measure the dilation of particles prepared at different initial volume fractions from relatively loose assemblies to densely packed ones. The samples consist of spherical marbles, plastic ellipsoids and tetrahedral dice at the centimeter scale and specially prepared particles at the millimeter scale. Under quasi-static shear, loosely packed samples compact while densely packed particles dilate, as in previous studies. For small shear amplitudes, both the dilation and compaction of the tetrahedral packings is significantly larger than that of spheres.

9:48AM Y13.00010 Dynamic crystallization in granular flow¹, ALINE HUBARD, MARK D. SHATTUCK, The City College of New York — We explore dynamic crystallization in simulations of two dimensional (2D) inelastic frictional hard disks as a model for granular materials. Previous simulations and experiments show formation of hexagonal structures in quasi-2D systems under vibration, rotation, and shearing. In experiments of a uniform but non-equilibrium steady-state (UNESS) under constant pressure the gas-crystal transition shows all of the classic signs of a first-order sublimation phase transition including discontinuous change in density, rate dependent hysteresis, and an equation of state consistent with sublimation. We use molecular dynamics to simulate steady shear under a variety of boundary conditions to determine a dynamic equation of state in the density range of the crystallization transition. We compare the dynamic equation of state with that found in non-flowing UNESS experiments, simulations, and theory.

¹Funding: National Science Foundation DMR-0934206, CBET-0968013.

10:00AM Y13.00011 The path to fracture: dynamics of broken-link networks in granular flows, MARK HERRERA, University of Maryland, SHANE MCCARTHY, STEVEN SLOTTERBACK, MICHELLE GIRVAN, WOLFGANG LOSERT, University of Maryland — Capturing the dynamics of granular flows on intermediate length scale can often be difficult. We propose the broken-links network as a new tool to study fracture at the intermediate scale. Using experimental data on the 3D tracks of all particles in a region, we calculate the dynamically evolving broken-links network and observe a second-order, percolation-like phase transition in the formation of the giant component as links are broken. We implement a velocity gradient model of link breakages and find that the model demonstrates a faster growth of the giant component than the data. Surprisingly, the broken-links network formed in the model is also more highly clustered than our empirical observations.

10:12AM Y13.00012 Hockey night in phase space, KIRI NICHOL, Leiden University, KAREN DANIELS, North Carolina State University — In order to explore the possibility of developing a statistical mechanics for dissipative ensembles, we have performed an experiment in which we track the translational and rotational velocities of pucks on an air hockey table. The pucks are driven by bumpers at the boundaries and are bidisperse to prevent crystallization. At packing fractions of 60% we find that the system distributes rotational and translation energy according to the equipartition theorem. However, as the packing fraction increases, the ratio of rotational energy to translational energy also increases to a value larger than predicted by equipartition. The translational and angular velocity distributions are approximately exponential and the distributions of the translational velocity are the same for both large and small particles. In contrast, the distribution of the angular velocities is broader for the small particles than for the large.

10:24AM Y13.00013 Rotational statistics in dense granular flows of smooth cylindrical particles, JEFFREY OLAFSEN, JACOB JANTZI, Department of Physics, Baylor University — We report the results of an experiment to investigate the dissipation in the rotational degree of freedom for smooth cylindrical particles in a dense, driven granular flow. The flow is studied in a rotating drum of radius $R = 30$ cm for particles of radius $r = 0.635$ cm while the cell is rotated at speeds between 0.25 and 0.75 Hz. The 2D geometry of the experimental design allows for the measurement of two translational degrees of freedom as well as the rotation of the disks within the driven flow. The rotational velocity statistics demonstrate non-Gaussian behavior as well as a significant amount of energy being dissipated within the flow via the tangential friction between the particles. The results of this experiment are significant in that many driven granular experiments use smooth cylindrical or spherical particles to investigate granular dynamics, but the contribution from the rotational degrees of freedom are often unmeasured. A novel imaging technique is used to extract both the translational and rotational velocity statistics to a high degree of precision in the entire cell during the experiment.

10:36AM Y13.00014 ABSTRACT WITHDRAWN —

10:48AM Y13.00015 Size Segregation of Granular Materials, ANURAG TRIPATHI, D.V. KHAKHAR, Indian Institute of Technology Bombay — Segregation of granular materials due to size difference while flowing/energized is a very well known but poorly understood phenomena. Despite of some good understanding of the mechanism of size segregation, predictive models for size segregation are not available. Size segregation of binary granular mixtures flowing over inclined plane is studied by means of DEM simulations. Buoyant force acting on trace particles of a bigger size is obtained by varying the density of the trace particles rising/sinking in the granular flow. We show that moderately big trace particles of same density as that of the light particles tend to rise because of higher buoyancy forces than the weight of the trace particles. For very big trace particles of same density, however, the buoyant force becomes smaller than the weight of the particles causing the particles to settle down. Drag force on the trace particle is found to be given by Stokes' law. Friction drag is found to almost 10 – 12% of the weight of the trace particles. Incorporating the Stokes' law and balancing the segregation and diffusion flux of big particles, we are able to predict the number fraction of the big particles in terms of viscosity and diffusivity for moderately dilute binary mixture of different size particles. The proposed theory is tested against DEM simulation results and very good agreement has been found with the simulation results.

Friday, March 25, 2011 11:15AM - 2:15PM —
Session Z9 DFD: Complex Fluids, Polymers, Gels D220

11:15AM Z9.00001 An anisotropic continuum model for flow, aggregation and microstructure evolution in magnetorheological fluids, MURAT OCALAN, GARETH MCKINLEY, Massachusetts Institute of Technology — The complexities associated with the transport of magnetorheological (MR) fluids under non-uniform magnetic and flow fields pose unresolved problems for generating accurate computational models. The evolutions of the electromagnetic and rheological properties of MR fluids are strong functions of the suspension microstructure; however, the geometrical features that lead to the field non-uniformities are often of a much larger length scale. To address these commonly occurring flow problems, we develop an anisotropic continuum model for MR fluids in which the electromagnetic stress is incorporated into the constitutive model for the viscoplastic stress generated in the bulk fluid by considering the generation and distortion of suspension microstructure under flow. The new model is incorporated into both a single-phase and a two-phase continuum description of the suspension. The aggregation dynamics and the evolution of MR fluid microstructure are observed in unique ferromagnetic microfluidic channels that replicate flow conditions of practical interest. The predictions of the newly developed models are verified with the experimental observations of microstructure evolution and macroscopic measurements of fluid rheology.

11:27AM Z9.00002 Electrorheological response of dense strontium titanate suspensions, CARLOS ORELLANA, JINBO HE, HEINRICH JAEGER, James Franck Institute and Department of Physics, The University of Chicago, Chicago, IL 60637, USA — Strontium Titanate (STO) particles were synthesized using a new method of precipitating the STO out of a water solution by adding alcohol. When dispersed in silicon oil, dense STO suspensions exhibit a high static yield stress in the presence of an electric field (200kPa at 5kV/mm), high shear stress at high shear rates and low current densities. We also find that the yield stress increases roughly linearly with applied field. This behavior is a key characteristic of a polar molecule dominated electrorheological effect. We also observed stress stiffening with time under low shear, stress oscillations, and stress reduction with strain. These effects can be accounted for by the interaction of permanent dipoles with the particles, the creation of shear bands of a few particles in width and the lack of self-diffusion in the samples.

11:39AM Z9.00003 Molecular Simulations of Particle Nanorheology, MIR KARIM, RAJESH KHARE — Over the past few years, experimental and theoretical developments in the field of microrheology have enabled determination of the local mechanical properties of complex materials. In this presentation, we will extend this approach to determine the local viscoelastic properties of polymeric materials using molecular dynamics (MD) simulations. Molecular simulations provide the unique ability to explicitly account for the intermolecular interactions in the system. Thus an approach based on molecular simulations allows for the determination of the viscoelastic properties at the nanoscale. The specific system that is studied in this work consists of a polymeric melt in which the polymers are modeled as bead-spring chains. We will present a comparison of the results obtained from the passive and the active nanorheology approaches. A discussion of the parameter (e.g. amplitude and frequency) ranges that allow usage of these techniques will also be presented.

11:51AM Z9.00004 Microscopic Approach for the Friction on a Spherical Particle in Dense Liquids: Hydrodynamics and Beyond, UMI YAMAMOTO, KENNETH SCHWEIZER, University of Illinois, Urbana-Champaign — We propose a new microscopic, non-mode-coupling, statistical dynamical approach to deriving the Stokes-Einstein (SE) friction coefficient of a large spherical particle dissolved in a dense fluid. The real space method is based on including as a slow variable the force exerted on a particle by the surrounding fluid. By exploiting the appropriate separation of time and length scales, and the Kirkwood superposition approximation for multi-point correlations, the SE result is obtained including the slip and stick limits plus the crossover function. This advance provides the foundation for developing a unified theory of friction for nanoparticles that includes both hydrodynamics and the non-hydrodynamic contribution associated with material-specific particle-fluid and particle-particle forces. Applications to nanoparticles in unentangled and entangled polymer solutions and melts, under various interfacial polymer-particle structure conditions, will be reported. Questions of particular interest include how the non-hydrodynamic friction contribution scales with particle radius, the role of length-scale-dependent viscosity in polymer liquids, and the conditions required for crossover to the hydrodynamics-dominated regime.

12:03PM Z9.00005 Rheology of bacterial flagella suspensions, SEVIM YARDIMCI, THOMAS GIBAUD, DANIEL CHEN, EDWARD BARRY, ZVONIMIR DOGIC, Physics Department, Brandeis University — The mechanical behavior of a suspension of rigid and semiflexible filaments has been studied in great detail. In comparison the effect of the filament geometry has been relatively unexplored. We present experimental results on the rheological behavior of suspensions of curly and straight flagella with an identical average contour length. We find that both suspensions are trapped in a glassy state and exhibit a solid-like behavior. We observe that the scaling of viscoelastic moduli is highly dependent on filament geometry. Taken together, this highlights the role of filament geometry in suspension mechanics.

12:15PM Z9.00006 Brownian Dynamics simulations of dilute graphene solutions under flow, YUEYI XU, MICAH GREEN, Department of Chemical Engineering, Texas Tech University — Many graphene-based materials (such as thin conductive films and nanocomposites) are processed in the liquid phase and require the conformation and alignment of graphene in solution to be precisely controlled. However, prior studies of conformation dynamics of sheetlike macromolecules such as graphene have been limited to equilibrium behavior, and there have been no studies of the dynamics of sheetlike macromolecules on flow processing timescales. Here we develop Brownian Dynamics (BD) algorithms in order to quantify the effects of flow processing on graphene conformation. The method is conceptually similar to those used for linear polymers; we coarse-grain the sheet using a bead-rod lattice of arbitrary 2-D connectivity and develop a novel theoretical framework for bending and metric forces. Using this technique, we simulate the conformation dynamics of dilute sheetlike macromolecule solutions in shear flow and compute the corresponding solution properties as a function of flow strength, sheet size, and solvent quality.

12:27PM Z9.00007 Orientation Dependent Gelation of Platelet Suspensions, YA-WEN CHANG, ANDRES MEJIA, ZHENG DONG CHENG¹, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77832 — Gelling behavior of colloidal suspensions of disk-shaped particles has long been used as an ideal system for studying the formation of arrested state of matter. High aspect ratio synthetic α -Zirconium phosphate (α -ZrP) monolayer platelets have recently received our attention as a new type of liquid crystal building blocks. We report the phase diagram of charged α -Zirconium phosphate platelet suspensions across the isotropic (I)–nematic (N) region versus salt concentrations. Typical electrostatic screening induced flocculation and gelation of platelet suspensions were observed. The morphological and rheological characteristics of liquid crystalline and colloidal gel phases were studied with polarized optical imaging and rotational/oscillatory rheometer. At high ionic strengths ($>10\text{mM}$), a re-entrance of fluidic liquid crystal phase occurs when particle volume fractions are above the arrested gel phase. We contribute this behavior to the competition between the driving forces for isotropic/nematic and sol/gel transitions of attractive colloidal platelets. Strong particle alignment hinders gelation, which usually demonstrates the “house of card” configuration in platelet suspensions; Isotropic suspensions flocculate and gel easily, as we confirmed experimentally.

¹Material Science and Engineering Program, Texas A&M University, College Station, TX 77832

12:39PM Z9.00008 Dynamic separation of macromolecules under temperature gradient¹, YUSUKE MAEDA, The Rockefeller University, Center for Studies in Physics and Biology, AXEL BUGUIN, Institut Curie, Centre de recherche, CNRS/UMR, ALBERT LIBCHABER, The Rockefeller University — Thermophoresis is a motion of suspensions in a fluid that are subjected to a temperature gradient. Although its effect is widely studied in case of single solute in water, little is known about how the mixture of different solutes is affected. We heated water with an infrared laser by $\Delta T_{\max}=5\text{C}$ and $\nabla T=0.25\text{C}/\mu\text{m}$ to induce thermophoresis of polyethylene glycol (PEG) and DNA. PEG is depleted from the hot region and results in a stationary gradient of its high volume fraction ϕ . Under this high concentration of PEG, DNA of small concentration is submitted to thermophoresis and osmotic pressure difference. The DNA shows regime of depletion, ring-like localization and accumulation as the volume fraction of PEG increases. As the osmotic force depends on the size of trapped solutes, DNA of different size accumulates at different regions. Depending whether the DNA size is below or above 5kbp a different scaling of position versus DNA size is observed. Thermal separation is a general phenomenon. It applies also to RNA and microbeads.

¹YTM is supported by JSPS fellowship and M.Josee-H.Kravis fellowship from the Rockefeller University.

12:51PM Z9.00009 Non-affine deformations in flexible and semi-flexible polymer gels¹, ANINDITA BASU, Physics and Astronomy, University of Pennsylvania, QI WEN, Institute for Medicine and Engineering, University of Pennsylvania, XIAOMING MAO, TOM LUBENSKY, Physics and Astronomy, University of Pennsylvania, PAUL JANMEY, Institute for Medicine and Engineering; Physics and Astronomy, University of Pennsylvania, ARJUN YODH, Physics and Astronomy, University of Pennsylvania — We test the validity of affine deformation assumption in flexible and semi-flexible polymer networks by embedding different-sized fluorescent tracer beads within model polymer networks and quantifying their displacements under shear. A conventional rheometer is used with a confocal microscope for this purpose. Non-affinity is quantified as a function of applied strain, polymer chain density, cross-link concentration, network morphology, reaction kinetics and size of probe particles used. Non-affinity measurements in flexible polymer gels are in qualitative agreement with current theories in rubber elasticity. For semi-flexible bio-polymer gels, measurements indicate that non-affine deformations are small for networks of thinner, relatively flexible filaments and get smaller as strain increases into non-linear elastic regime. These small measures are consistent with the entropic model for non-linear elasticity of semi-flexible gels. However, as filament stiffness and mesh size increase, the deformations become more non-affine, as predicted by the enthalpic bending and stretching models of non-linear elasticity.

¹MRSEC DMR-0520020, DMR-0505048, and DMR- 0079909

1:03PM Z9.00010 Drying of polymer films: study of demixing phenomena, JULIE FICHOT, RODOLPHE HEYD, CNRS, MARIE-LOUISE SABOUNGI, CHRISTOPHE JOSSEREND, EMILIE COMBARD, JEAN FRANCOIS TRANCHANT — Understanding the mechanisms that control the stability of polymeric films is important in beauty care. We have prepared films starting from a water-soluble organic polymer, a preservative and water. We study the drying of these films as a function of several physicochemical parameters that control their interfaces such as temperature, humidity and the nature of the support. The viscoelastic properties of the solutions before spreading out are analyzed with a rheometer in order to adjust the temperature. The topography of the films is observed by optical microscopy and the evolution of the drying is determined with a precision gravimetric balance. The behavior of the films on a nanometric scale is followed by AFM. During the drying process, droplets appear on the surface of the film, made up of water surrounded by a shell of preservative. As the films dries, the water evaporates from the droplets and the preservative spreads on the surface of the film, leading to the formation of craters on the surface of the dried film. The dimensions and numbers of the craters depend strongly on the type and concentration of the preservative employed.

1:15PM Z9.00011 Multiple Particle Collision Dynamics Simulations of the Effect of Catenation on the Structural and Dynamic Properties of Ring Polymers in Solution, GOVIND HEGDE, RAJESH KHARE, Department of Chemical Engineering, Texas Tech University — Multiple particle collision dynamics (MPCD) is a particle based mesoscale simulation technique that coarse-grains the solvent while preserving the hydrodynamics, thus enabling simulations over longer length and time scales as compared to molecular dynamics (MD) simulations. In this work, MPCD is used to study the effect of topology on the structural and dynamic behavior of complex fluids. The systems of interest in this work are the dilute solutions of ring and catenated ring polymers. MPCD simulation results are compared with those obtained from MD simulations in which the hydrodynamic interactions are governed by the explicit intermolecular interactions. Different chain topologies are considered such as catenated as well as multi-catenated rings. Results will be presented for the effect of chain length on the radius of gyration and chain diffusion coefficient for the various topologies studied. Our results will also be compared with previous theoretical and experimental work reported in literature.

1:27PM Z9.00012 Strongly anisotropic polymer networks, STEPHAN ULRICH, University of Goettingen, ANNETTE ZIPPELIUS, University of Goettingen, Max Planck Institute for Dynamics and Self-Organization, PANAYOTIS BENETATOS, Cavendish Laboratory, University of Cambridge — We investigate a network of worm-like chains, which are strongly oriented along a preferred direction due to an external field, boundary conditions, or a nematic environment. We discuss the effects of random permanent cross-links, whose density may follow an arbitrary distribution along the alignment direction. We show that the tilt modulus is unaffected by cross-links. As the cross-link density is increased beyond the gel point, the network develops a stiffness to in-plane shear deformations. Results for the shear elasticity and fluctuations of the polymer chains are presented. The case of cross-linking the chains on one end only is highlighted, it constitutes a simple model for polymer brushes. Moreover force-extension curves are presented for a toy model that consists of two cross-linked chains.

1:39PM Z9.00013 Structure and Dynamics of Water Absorbed in Polyamide, MARCO LAURATI, PAUL SOTTA, DIDIER LONG, LUDOVIC ODONI, VERONIQUE BOSSENEC, THIERRY BADEL, Laboratoire Polymeres et Materiaux Avances, UMR5268, CNRS/Rhodia Recherches et Technologies, 85 Rue des freres Perret, 69192 Saint-Fons Cedex, ARANTXA ARBE, ANGEL ALEGRIA, JUAN COLMENERO, Centro de Fisica de Materiales (CSIC-UPV/EHU), Paseo Manuel de Lardizabal 5, 20018 Donostia/San Sebastian, Spain — We present results of elastic and inelastic neutron scattering, dielectric spectroscopy and MD simulations concerning the structural organization and the dynamics of water absorbed in an amorphous polyamide material. We find that, different from predictions of available models of water absorption in polyamide, only a small fraction of water binds to the amide groups while most of it organizes into aggregates. Such structural model is supported by results on the microscopic dynamics of water, which can be described as diffusive motions with a relaxation time following a VFT dependence on temperature, similarly to bulk water. Measured average diffusion coefficients of water absorbed in Polyamide are approximately two orders of magnitude smaller than in bulk water, revealing the confinement effect of the polymer matrix.

1:51PM Z9.00014 Order parameter defining liquid-liquid transition in water¹, J. RAUL GRIGERA, OSVALDO CHARA, ANDRES MCCARTHY, IFLYSIB (UNLP-CONICET), c.c. 565, La Plata, Argentina — Water presents both open tetrahedral and compact hexagonal structures. Although several order parameters have been proposed to quantify this, all of them are only applicable to data produced by simulation. We present an order parameter (P_r) that is calculated from the radial distribution function $g(r)$, also available from experiment. We hereby extract the tetrahedral and hexagonal components from the $g(r)$, each one reconstructed as the sum of a Freundlich distribution for the first peak, two subsequent Gaussian distributions, and a sigmoidal to account for the rest. The order parameter can be calculated from the relative contribution of tetrahedral over hexagonal contribution. We obtained the P_r for SPC/E water model from molecular dynamics simulations of water at different pressures and temperatures. At 300K, the pressure in which both, tetrahedral and hexagonal contributions become equal ($P_r=0$), a structural crossover is found in the vicinity of 2kbar, close to the pressure at which the "anomalous" behavior manifests. Having computed P_r for this wide range of pressure and temperature we then calculate the HDL spinodal, the coexistence line, the second critical point, and the Widom line.

¹Supported by CONICET, UNLP, and CIC Prov.BsAs.

2:03PM Z9.00015 Particle and fluid diffusivity of non-colloidal suspensions, EMMANOUELA FILIPPIDI, ALEXANDRE FRANCESCHINI, CHUI-LAI CHEUNG, JACOB TUTMAHER, SEAN PARADISO, TARUN JAIN, DAVID PINE, Center for Soft Matter Research, New York University — Suspensions of non-colloidal spheres at moderate volume fractions (0.2-0.4) under slow periodic strain undergo a phase transition from an absorbing to an active fluctuating state. Particle trajectories change from reversible below the critical strain to irreversible above. We measure the fluid diffusivity of the fluorescently labelled fluid and compare it with the particle diffusivity in order to obtain a measure of the coupling between the two. Of particular interest is how the fluid diffusivity changes near the onset of irreversibility of the particle trajectories.

Friday, March 25, 2011 11:15AM - 2:15PM – Session Z13 GSNP DFD: Granular Materials II D225/226

11:15AM Z13.00001 Perfect fluid flow from the impact of a dense granular jet, WENDY W. ZHANG, JAKE ELLOWITZ, NICHOLAS GUTTENBERG, University of Chicago, HERVE TURLIER, Institut Curie, SIDNEY R. NAGEL, University of Chicago — Axisymmetric collision of a cylindrical water jet with a circular target generates a thin conical sheet, also known as a water bell [Cheng et al. Phys. Rev. Lett. 99, 2007]. Intriguingly, recent experiments on granular jet impact in the regime of dense inertial flow reveal similar behavior: the angles by which the collimated sheets of particles are ejected from the target agree closely with the angles measured in the water-bell experiments [Clanet, C. J. Fluid Mech. 430, 2001]. This quantitative correspondence suggests that the collective granular motion during impact can be modeled as an incompressible, continuum fluid. Since viscous effects are weak in water-jet impact and the granular jet is comprised of non-cohesive particles (hence possessing zero surface tension), the simplest scenario is that the continuum motion corresponds to the flow of a perfect fluid. We show an exact solution of 2D perfect fluid impact agrees quantitatively with 2D discrete-particle simulation results. Therefore, the emergence of a highly collimated outgoing sheet does not necessarily signal the creation of a thermodynamic liquid phase. Such a coherent outcome results generically when the motion is nearly incompressible and dominated by inertia.

11:27AM Z13.00002 Jet-Induced Granular 2-D Crater Formation with Horizontal Symmetry Breaking¹, ABE CLARK, ROBERT BEHRINGER, Duke Physics — We investigate the formation of a crater in a 2-D bed of granular material by a jet of impinging gas, motivated by the problem of a retrograde rocket landing on a planetary surface. As the strength and height of the jet are varied, the crater is characterized in terms of depth and shape as it evolves, as well as by the horizontal position of the bottom of the crater. The crater tends to grow logarithmically in time, a result which is common in related experiments. We also observe an unexpected horizontal symmetry breaking at certain well-defined conditions. We present data on the evolution of these asymmetric states and attempt to give insights into the mechanism behind the symmetry-breaking bifurcation. This horizontal symmetry breaking is highly suggestive of a pitchfork bifurcation, and we give evidence to classify it as forward or backward in different regimes of operation. As we will demonstrate, the formation of an asymmetric crater could be of considerable practical concern for lunar or planetary landers, particularly in the case of a backward pitchfork bifurcation, which is characterized by hysteresis and very rapid transitions.

¹supported by ORBITEC (contract # OTC-GS-02381), subcontracted from USAF (contract # NNX09 CF72P) and by NASA contract

11:39AM Z13.00003 Simulations of granular jet impact deadzone formation, NICHOLAS GUTTENBERG, JAKE ELLOWITZ, WENDY ZHANG, University of Chicago, HERVE TURLIER, Univ. Pierre & Marie Curie, SIDNEY NAGEL, University of Chicago — Motivated by granular experiments showing the emergence of continuum-like dynamics when a dense jet hits a target, we simulate the impact of 2D and 3D granular jets of frictional, cohesion-less grains upon a fixed target. This is an inertial, dense jet regime where the motion is essentially incompressible. Impact deflects the material in the jet into a hollow conical sheet. The cone angles measured in simulation are consistent with previous experimental studies of the 3D granular jet impact. In addition, experiments have revealed the formation of a "dead zone," a region where the grain motion is negligibly small. The simulation shows that this dead zone can only form when a no-slip boundary condition is enforced at the target. The presence or absence of the dead zone leads to a change in cone angle consistent with the experimentally observed differences in cone angle between the 3D granular flow and the corresponding water bell flow.

11:51AM Z13.00004 Endless penetration in impact cratering¹, J. CARLOS RUIZ-SUAREZ, Cinvestav-IPN, Unidad Monterrey, FELIPE PACHECO-VAZQUEZ, Cinvestav-IPN, Unidad Merida, J. MANUEL SOLANO-ALTAMIRANO, Cinvestav-IPN, Unidad Monterrey, GABRIEL CABALLERO-ROBLEDOS, Cimav-Unidad Monterrey — The phenomena of impact cratering have been in the minds of physicists at least for two decades; the reason being the interest for elucidating the intriguing rheological response produced by granular systems when they are penetrated. With the great amount of work done in this regard, one could think that the problem is reasonably well understood. However, we study here a fascinating phenomenon never observed before in granular penetration experiments: depending on the mass of a projectile colliding onto a granular bed, it either stops at a given depth like normally expected, or keeps sinking with a terminal velocity as if the medium were a newtonian fluid. Understanding this intriguing behaviour could help us to know the subtleties of intrusion phenomena in granular media.

¹Grant 101384, Conacyt México

12:03PM Z13.00005 Avalanches of Singing Sand in the Laboratory, SIMON DAGOIS-BOHY, Kamerlingh Onnes

Laboratorium, Universiteit Leiden, SYLVAIN COURRECH DU PONT, STÉPHANE DOUADY, Laboratoire M.S.C., Univ. Paris Diderot — The song of dunes is a natural phenomenon that has arisen travellers' curiosity for a long time, from Marco Polo to R.A. Bagnold. Scientific observations in the XXth century have shown that the sound is emitted during a shear flow of these particular grains, the free surface of the flow having coherent vibrations like a loud speaker. The sound emission is also submitted to a threshold effect with many parameters like humidity, flow speed, surface of the grains. The sound has been reproduced in laboratory avalanche experiments close to the natural phenomenon on field, but set in a channel with a hard bottom and a few centimeters of sand flowing, which contradicts explanations of the sound that involve a sand dune under the avalanche flow. Flow rates measurements also show the presence of a plug region in the flow above the sheared band, with the same characteristic length as the coherence zones of the sound. Finally we show experimentally that the Froude number, once modified to take into account the height of this plug band, is the parameter that sets the amplitude of the sound, and produces a threshold that depends on the grain type.

12:15PM Z13.00006 Shear strength of vibrated granular/granular-fluid mixtures, BRIAN UTTER,

RALPH HERMAN, BEN FOLTZ, James Madison University — The behavior of dense granular materials can be characterized by the continuous forming and breaking of a strong force network resisting flow. This jamming/unjamming behavior is typical of a variety of systems and is influenced by factors such as grain packing fraction, applied shear stress, and the random kinetic energy of the particles. We present experiments on shear strength of granular and granular-water mixtures under the influence of external vibrations, one parameter that leads to unjamming. We use low vibration ($< 1g$) and slow shear and measure avalanching statistics in a rotating drum and the torque required to move a stirrer through a sand/water mixture. We find that external vibration (i) increases granular strength at small vibrations in the dry system, (ii) removes history dependence (memory), and (iii) decreases shear strength at all accessible saturation levels in the sand-fluid system. Additionally, shear strength is found to be smallest for both dry and completely saturated mixtures. Additional ongoing experiments probe beyond a dimensionless acceleration of 1 and explore jamming and surface chemistry effects in the avalanching flow of granular/fluid mixtures.

12:27PM Z13.00007 Collisions between solitary waves in granular alignments¹, SURAJIT SEN, SUNY

Buffalo, DIANKANG SUN, New Mexico Resonance — Solitary waves arise naturally when an unloaded alignment of elastic spheres, that is held between fixed end walls, is perturbed at one end. Unlike most known classes of solitary waves, those in granular materials are special and tend to break down and reform during any collision. Here we present what happens when two solitary waves of unequal magnitude suffer head-on and overtaking types of collisions. We will show that these collisions provide ways for solitary waves to not only become smaller but also become larger (within bounds) and that they are the underlying reason behind the emergence of the quasi-equilibrium phase.

¹Research Support: Army Research Office

12:39PM Z13.00008 Oil in Water Emulsion Flow in a 2D Hopper¹, XIA HONG, DANDAN CHEN, KENNETH

DESMOND, ERIC WEEKS, Physics Dept., Emory University — Granular flows are still somewhat poorly understood. One such case is the flow of 2D disks through a hopper. In a prior experiment by To (K. To, et al. PRL 86(1) 2001), they found that as 2D disks flow through a hopper they may jam due to arch formations at the hopper exit, and that the jamming probability can be increased by enhancing the static friction between the disks. In our study we remove the effects of static friction by using quasi-2D oil in water emulsion droplets flowing through a hopper to understand the role of friction in jamming. The droplets feel a viscous friction, but no static friction. Similar to the granular experiment, our oil droplets flow due to gravity. We have observed the transition between jammed and unjammed flows in our setup, and we are currently investigating its nature as the hopper size changes. In our experiments, jamming seems to occur only for very small hopper openings, and arches are always unstable.

¹the Petroleum Research Fund (47970-AC9)

12:51PM Z13.00009 Water Retention of Mixed Hydrogel Particles and Sandy Soil, YULI WEI,

DOUGLAS DURIAN, University of Pennsylvania — We study the water-holding capacity of mixed hydrogel particles and a model sandy soil. To probe static behavior, we develop a custom pressure plate method that measures the expelled water per unit pressure increment per unit cross-sectional area; results are analyzed in terms of the water-accessible pore areas in the granular packing. To probe dynamic behavior, we build a raindrop impingement set-up that measures the retained water inside a dry granular packing during steady rain at a fixed rate. The percentage saturation of the granular packing is deduced. In both studies, we first determine the influence of the packing height and then of the gel concentration and size. Results from pressure plate method show that the swollen hydrogel particles partially clog the pores in the sandy soil, so that less water could be expelled for a given pressure increment. The total water-accessible area determined from the expelled water curve decreases exponentially as the gel concentration increases. Large hydrogel particles are less efficient in clogging the pores when no extra confinement is applied on the packing. Results from the raindrop impingement measurements also show that the water-holding capacity of sandy soil is improved by addition of hydrogel particles.

1:03PM Z13.00010 Granular “electrophoresis”: in situ measurement of charge and size of freely-falling grains, SCOTT WAITUKAITIS, The University of Chicago, GUSTAVO CASTILLO, Universidad de Chile, SEBASTIAN GONZALEZ,

University of Twente, HEINRICH JAEGER, The University of Chicago — We present measurements of tribocharged, chemically identical grains falling from a hopper. Tribocharging is the transfer of electrical charge between contacting surfaces. Granular interactions are governed by contacts, and not-surprisingly tribocharging can have important effects on bulk granular behavior. What is surprising is that this occurs even in grains of the same material. Typically same chemistry tribocharging (SCT) correlates with the particle size distribution: larger particles charge positively and smaller particles negatively. However, the detailed mechanism of SCT remains elusive. We have developed an experimental technique to make *in situ* measurements of the particle size and charge on small (~ 100 - $500 \mu\text{m}$) grains. With high speed videography of freely-falling grains we resolve particle sizes down to a few microns, charges as small as a few thousand electrons, and forces as small as a few picoNewtons. Our results confirm the qualitative charge segregation observed in previous SCT experiments and provide quantitative measurement for theoretical comparison.

1:15PM Z13.00011 Strain-stiffening in random packings of granular chains, HEINRICH JAEGER, ALICE

NASTO, DYLAN MURPHY, ERIC BROWN, University of Chicago — We report on triaxial compression experiments performed to characterize the mechanical response of random packings of granular particles. For a wide variety of particle shapes, the packings yield when the shear stress exceeds a value on the order of the confining pressure. In contrast, granular chains consisting of flexibly connected beads exhibit strain stiffening (i.e., the effective modulus increases with strain), sustain stresses far beyond the confining pressure, and do not yield until the chains break. The critical chain length required for significant strain-stiffening to occur corresponds to the minimum circumference of closed loops the chains are able to form during the formation of the packings. This strain-stiffening behavior is similar to that found in polymer materials, and chain packings therefore may serve as a model system to quantify the contribution of pure entanglement effects to the strength of polymer materials in the absence of Brownian motion.

1:27PM Z13.00012 Anisotropic diffusion of vibrated semi-flexible granular rods, VIKRANT YADAV, ARSHAD KUDROLLI, Clark University — We discuss the diffusive dynamics of semi-flexible granular rods as a function of their concentration in a vertically vibrated container. These rods are composed of short beaded chains and are tracked with a camera, and their trajectories used to analyze the rotational and translational displacement as a function of area fraction ϕ . We observe that the diffusion in the parallel and perpendicular direction in the body frame of reference deviate from those calculated for thermally excited elastic polymer rods. In particular we find that the diffusion perpendicular to the major axis in dilute regime is observed to be greater than that in the parallel direction due to rotation about the major axis of the rod. The motion is observed to become sub-linear above $\phi = 0.48$ and 0.54 in the perpendicular and parallel directions, respectively, both lower than for spherical particles. Rotational diffusion is also investigated and found to deviate systematically from exponential decays with increase in ϕ .

1:39PM Z13.00013 Vibrofluidized melting of geometrically cohesive granular media, NICK GRAVISH, GEOFFREY RUSSELL, Georgia Tech, SCOTT V. FRANKLIN, Rochester Institute of Technology, DAVID HU, DANIEL I. GOLDMAN, Georgia Tech — Dry granular media composed of particles of special shapes (e.g. long rods or c-shaped particles) can display cohesive effects through particle geometry alone. We study the solid to gas transition in piles of c-shaped particles under vertical vibration as we vary acceleration and frequency. A cylindrical solid of particles is formed with wall angles near 90° and is placed on a solid surface. For fixed frequency as acceleration increases, the pile undergoes two transitions. The first is from the solid-like state to a liquid-like state in which the wall angles relax but the mobile particles remain spatially localized. The second is from the liquid-like state to the gaseous state in which particles become separated (not entangled). Using video and accelerometer measurements, we record the temporal evolution of the spatial density and pile-plate collisional impulse. A critical energy scale, set by the particle geometry and gravitational potential energy, governs the liquid-gas transition.

1:51PM Z13.00014 Switchable capillary bridges in sphere packings, CHRISTOPH GÖGELEIN, MARTIN BRINKMANN, MATTHIAS SCHRÖTER, STEPHAN HERMINGHAUS, Max-Planck-Institute for Dynamics and Self-Organization — If one adds a small amount of water to a heap of sand, it becomes paste-like since the grains get interconnected by capillary bridges. Due to this effect, we can easily sculpture wet sand (e.g., building a sand castle), whereas a heap of dry grains ripples away and cannot sustain any shape. In the present work, we use a non-Brownian suspension of glass spheres immersed in a binary liquid mixture. The suspending water-lutidine mixture exhibits a well studied lower critical point slightly above ambient temperature. Hence, the mixture starts to phase separate upon heating. Since the water-rich phase wets the hydrophilic glass spheres, capillary bridges are formed between adjacent particles. If the system is cooled below the demixing temperature, the bridges disappear within a few seconds by intermolecular diffusion. Thus, this systems offers the opportunity to switch the capillary bridges on and off by altering the temperature. In this presentation, we will show the temperature-induced formation of capillary bridges using confocal and bright light microscopy [1]. Furthermore, we will discuss the effect of capillary bridges on random sphere packings using a fluidized bed setup.

[1] C. Gögelein, M. Brinkmann, M. Schröter, and S. Herminghaus, *Langmuir* 26 (2010) 22, 17184.

2:03PM Z13.00015 Stable Solitary Waves in Granular Alignments¹, YOICHI TAKATO, SURAJIT SEN, SUNY Buffalo — We study the propagation of an impulse in a loaded chain of elastic spheres where the spheres are held between fixed walls. We show that for a certain critical loading, propagating impulses develop into solitary waves and these solitary waves are not measurably affected by wall collisions, the latter being typically the case with granular solitary waves. The properties of these special solitary waves and of possible connections between this problem and the Fermi-Pasta-Ulam problem will be addressed.

¹Supported by Army Research Office