



IRTG 1524

Spring School 2017

„Self-Assembly in Soft Matter Systems“

Beverly, MA, U.S.A.

March 05–11, 2017



THE UNIVERSITY
of NORTH CAROLINA
at CHAPEL HILL



TRIANGLE
MRSEC | Materials Research Science
and Engineering Center



Program

Sunday, March 05	
tba	Shuttle bus BOS airport → Wylie Inn
7:00 pm	Get together (reception)
8:00 pm	Dinner

Monday, March 06	
7:00 am	Breakfast
8:30 am	Coray M. Colina In silico synthesis and characterization of amorphous materials
9:30 am	William Ducker Surface Forces: Calculation and Measurement
10:30 am	Break
10:45 am	William Ducker Surface Forces: Measurement of the Hydrophobic Force, and Development of Surfaces to Prevent Bacterial Adhesion
12:00 pm	Lunch
1:00 pm	Preparation Round Table Discussion I (all groups)
3:00 pm	Break
3:30 pm	Poster introductions (#1–15)
5:00 pm	Spare Time
7:00 pm	Dinner
8:00 pm	Poster Session I (#1–15)

Tuesday, March 07	
7:00 am	Breakfast
8:30 am	Coray M. Colina pySIMM, nuSIMM and polymatic: in silico tools for the synthesis and characterization of amorphous materials
9:30 am	Bhuvnesh Bharti Assembly, structuring, and active motion in colloidal dispersions: Electrostatic interactions
10:30 am	Break
10:45 am	Bhuvnesh Bharti Assembly, structuring, and active motion in colloidal dispersions: External field induced interactions
12:00 pm	Lunch
1:00 pm	Preparation Round Table Discussion II (all groups)
3:00 pm	Break
3:30 pm	Poster introductions (#16–29)
5:00 pm	Spare Time
7:00 pm	Dinner
8:00 pm	Poster Session II (#16–29)

Wednesday, March 08	
7:00 am	Breakfast
8:30 am	Thomas Zemb Introduction to solvation-entropy driven weak aggregation: I. Pre-nucleation clusters of hydrated electrolytes
9:30 am	Break
9:45 am	Andreas Heuer Non-linear driving of particles in disordered systems: a potential energy landscape perspective

10:45 am	Career Opportunities
12:00 pm	<i>Lunch</i>
12:45 pm	Departure Shuttle/Sightseeing Tour Boston
5:00 pm	Spare Time
7:00 pm	Shuttle Departure (Boston)
8:00 pm	<i>Dinner</i>

Thursday, March 09	
7:00 am	<i>Breakfast</i>
8:30 am	Thomas Zemb II. Ternary mixtures containing hydrotropes with microemulsion-like properties
9:30 am	Andreas Heuer Shearing of glasses and supercooled liquids & Frame-guided assembly of amphiphilic molecules
10:30 am	<i>Break</i>
10:45 am	Margarida Telo da Gama Wetting of liquid crystals at structured substrates: statics and dynamics
12:00 pm	<i>Lunch</i>
1:00 pm	Poster Session (all posters) – Poster Voting
2:00 pm	Round Table Discussion I (groups A/C/D)
4:00 pm	<i>Break</i>
4:30 pm	Round Table Discussion I (groups A/C/D)
6:30 pm	Spare Time
7:00 pm	<i>Dinner</i>

Friday, March 10	
7:00 am	<i>Breakfast</i>
8:30 am	Margarida Telo da Gama Nematic films at structures surfaces: anchoring transitions and elastic instabilities
9:30 am	Bradley D. Olsen Swelling and Mechanics of Polymer Networks
10:30 am	<i>Break</i>
10:45 am	Bradley D. Olsen Effect of Defects on the Properties of Polymer Networks
12:00 pm	<i>Lunch</i>
1:00 pm	Spare Time
2:00 pm	Round Table Discussion II (groups B/E/F)
4:00 pm	<i>Break</i>
4:15 pm	Round Table Discussion II (groups B/E/F)
5:15 pm	Poster Prize Award/Feedback
6:00 pm	Spare Time
7:00 pm	<i>Dinner</i>

Saturday, March 11	
7:00 am	<i>Breakfast</i>
tba	Shuttle bus → BOS airport

Lecture Abstracts

Coray M. Colina

Department of Chemistry – University of Florida, Gainesville, FL, USA

I. In silico synthesis and characterization of amorphous materials

One of the most efficient methods for characterizing microporous materials is using computer simulations because they offer an attractive way to evaluate large number of materials rapidly and economically. In general, the construction of amorphous materials (e.g. amorphous polymer, hypercrosslinked polymers) *in silico* is quite challenging due to the lack of a reference structure (X-ray crystallography) and the nature of unfavorable energy from steric effects as a function of chain length. Several approaches have been attempted to generate the amorphous network structures such as assuming ordered structures or combination of smaller network fragments which are not ideal for many scenarios such as highly crosslinked amorphous systems. Currently, the state-of-the-art approach for construction of amorphous polymers is by simulated polymerization. In simulated polymerization, the approach involves energy minimization and molecular dynamics (MD) simulations as new bonds form throughout the synthesis process. By incorporating MD during polymerization and crosslinking, the system is allowed to equilibrate into a more favorable energy state and a more realistic structure can be obtained. The power and usefulness of this methodology is its predictive capability and general applicability, demonstrated, in this talk, for a representative group of polymers. Validation of the methodology is provided by characterization of the simulated structures in excellent agreement with available experimental data produced from our experimental collaborators and others, including densities, wide-angle X-ray scattering, surface areas, pore-size distributions, and adsorption isotherms. Systems to be discussed include:

1. Linear rigid PIMs: Backbone functionality
2. Design of Organic Molecules of Intrinsic Microporosity (OMIMs)
3. Hypercrosslinked polymers and
4. Molecular layer-by-layer polymerization.

II. *pySIMM*, *nuSIMM* and *polymatic*: in silico tools for the synthesis and characterization of amorphous materials

There is a great need for new easy-to-use applications to perform computational studies of amorphous (polymeric) materials. Whether the goal is to educate new researchers or expand accessibility to purely experimental researchers, one prohibitive hurdle is often the time spent learning the intricacies associated with complex simulation packages or high performance computing techniques. In this talk we will discuss the capabilities of three simulation tools (*nuSIMM*, *pysimm*, *polymatic*) designed to facilitate the structure generation, simulation and characterization of molecular systems. In general, polymeric material properties depend greatly on the specifics of each polymeric sample such as the molecular weight distribution, degree of branching, network structure, tacticity and monomeric composition. Examples showing the use of the different tools, including the development of a new computational polymer growth algorithm using *pysimm* designed to control molecular weight and build copolymers will be provided.

nuSIMM, new to molecular simulations (<https://nanohub.org/resources/nusimm>), is a web application powered by the open-source molecular simulation platform *pysimm* and built on the NSF funded cloud computing platform provided by nanoHUB which was designed to make performing molecular simulations easier. Cloud computing tools on nanoHUB can be accessed using any modern web browser. Input for simulation tools are collected through a graphical user interface in your browser and sent to computers in the cloud which perform simulation, collect results, and display results back in your web browser with the option of downloading data to analyze on your own machine. Simulation sessions can also be shared

between users to help facilitate collaboration and educate new researchers about simulation techniques without requiring users to have extensive knowledge about high performance computing.

polymatic (<https://nanohub.org/resources/17278>) Polymatic is a set of codes for structure generation of amorphous polymers by a simulated polymerization algorithm. The main task of Polymatic is to perform polymerization steps within a system based on a number of defined bonding criteria. It works in conjunction with a simulation package to perform energy minimization and molecular dynamics simulations during the polymerization.

pySIMM (<http://pysimm.org>) short for python simulation interface for molecular modeling, is a python package that provides a collection of different simulation tools while offering smooth integration with highly optimized third party software for specialized tasks. The platform provided by *pysimm* has helped the rapid development of new molecular modeling applications specifically in the area of amorphous polymeric systems, an area that can benefit greatly from more simulation tools. The modular tools in the *pysimm* package provide a toolbox for researchers to build applications with complex workflows through easy to use functions and fully object oriented representations of molecular systems. *pysimm* interfaces with existing software, such as the LAMMPS simulation package and *polymatic* to perform expensive or highly specific computations.

Notes:

William Ducker

Department of Chemical Engineering – Virginia Tech, Blacksburg, VA, USA

Surface Forces:

I. Calculation and Measurement

The short-range forces that are dominated by thin surface layers, “Surface Forces”, are important in many natural phenomenon (e.g. adhesion of cells and wetting) as well as in the production and use of man-made products (e.g. oil refining, protective coatings, and colloidal food products). This tutorial will begin with a brief description of applications and the relationship between surface forces and colloidal stability, and then describe the calculation of surface forces. Calculation will consider the total force to be the sum of various components, the van der Waals force, double-layer force, hydration, hydrophobic, depletion, polymer forces etc. The final part of the tutorial will describe the measurement of surface forces using atomic force microscopy.

II. Measurement of the Hydrophobic Force, and Development of Surfaces to Prevent Bacterial Adhesion

This talk will discuss two research topics related to surface. The first talk part will discuss rather pure research on the measurement of hydrophobic forces and the second will discuss rather applied research on bacterial adhesion.

Hydrophobic forces: Thirty years ago there was considerable excitement over the first report of a long-ranged “hydrophobic force” between solids that were not wet by water [Israelachvili and Pashley, *Nature* **1982**, *300*, 341-342]. Of particular importance is the question of the range of the force: a “hydrophobic force” is distinct from molecular-length adhesion that may contribute to adhesion. I describe careful measurements of the forces between smooth and carefully controlled hydrophobic surfaces to examine whether there is a force, beyond that expected for van der Waals and double-layer forces, between hydrophobic surfaces.

Bacterial Adhesion. The adhesion of bacteria to surfaces is a major cause of sickness and death. One important aspect is the adhesion of bacteria to devices that are placed inside the body during medical procedures or as long-term implants that may be the source of an infection or the site of growth. In this section I will discuss our efforts to modify surfaces that are robust in the “dirty” world of real devices.

Possible topics for discussion

1. Comparison of surface forces measurement techniques: what are the conditions when various methods are method best applied?
2. Are the components of surface forces additive?
3. Can surface forces be predicted from the properties of **isolated** surfaces?
4. Importance of the rate of measurement: response time of intervening fluid and surface.
5. Suitability of approach: when is it sensible to predict surface forces; when can one predict properties from surface forces?

Notes:

Bhuvnesh Bharti

Cain Department of Chemical Engineering – Louisiana State University, Baton Rouge, LA, USA

Assembly, structuring, and active motion in colloidal dispersions:

I. Electrostatic interactions

Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

The multiscale self-assembly of atoms, molecules, and particles is the origin of all physical mesoscopic matter. The spatial organization, symmetry, and physical properties of the assembled matrices are determined by the characteristics of interparticle interactions. In this lecture I will focus on fundamentals of electrostatic interactions in colloidal dispersions. I will discuss the origin, mode of operation, and implication of charge-charge interactions on colloidal assembly. These fundamentals will be applied to study the heteroaggregation of silica-lysozyme, and polystyrene particles. The kinetic, and thermodynamic aspects of aggregate morphology and structure formation will be explored. I will also present the effect of surface charge density, screening length, and bulk concentration on the aggregate structure. Application of advanced characterization techniques such as small angle x-ray scattering, analytical centrifugation, and microscopy (electron, and light) to particle-structure elucidation will be presented within the scope of colloidal-aggregation.

II. External field induced interactions

Assembling colloidal particles presents a challenging and interesting research area for development of patterned and ordered colloidal structures. The most popular and widely used technique for tailoring ordered structures is the application of an external field (electric or magnetic) to the colloidal dispersions. In this lecture, I will discuss how external fields can be used to assemble permanent linear chains, 2D crystals, and transitory particle networks. The origin of field induced interparticle interactions, and the effect of various field parameters on local structures will be presented. In addition to the assembly of isotropic particles in external fields, I will present directional active motion of Janus colloids in high frequency AC-electric field, termed as Induced Charge Electrokinetic Phenomenon (ICEP). The origin of the particle motion, and its effect on multiparticle colloidal assembly will be discussed. The understanding developed for the single particle active motion will be extended to the migration and translocation of multiparticle cluster, which show much more complex motion in 3D space.

Notes:

Thomas Zemb

Institut de Chimie Séparative de Marcoule, France

Introduction to solvation-entropy driven weak aggregation

I. Pre-nucleation clusters of hydrated electrolytes

Pre-nucleation clusters of cations, with mixed anions and hydroxide, and wet by water, are present in the stability phase diagram of inorganic electrolytes, in between the classical domains of simple mono-cation «complexes» and the continuous hydroxide solid that is contained in the classical pH-EH phase diagrams used in inorganic chemistry. Since 2008, the inorganic chemistry doxa has been put upside down by unambiguous detection of these pre-nucleation clusters, that have been labelled DOLLOPS. After nearly ten years, more than hundred papers describe this emerging field of weakly bound colloids. Pre-nucleation amorphous clusters, as DOLLOPS, are an inorganic analogue of pre-micelles known for short chain amphiphiles, and probably also a precursor in the formation of meso-materials. Classical nucleation theory, as well as established concepts of spinodal decomposition and liquid-liquid demixing, should be extended via the recently proposed pre-nucleation cluster pathway. The features of pre-nucleation clusters are presented and discussed in

relation to recent modifications of the classical and established models for phase separation, together with a review of experimental work and computer simulations on the characteristics of pre-nucleation clusters of calcium phosphate, calcium carbonate, iron(oxy)(hydr)oxide, silica and also amino-acids. The role of pre-nucleation clusters as solute precursors in the emergence of a new phase will also be described.

Reference:

DOI: 10.1039/c3cs60451a; Denis Gebauer et al. : *Chem. Soc. Rev.*, 2014, **43**, 2348

II. Ternary mixtures containing hydrotropes with microemulsion-like properties

The concepts “hydrotrope” and “hydrotropy” are reviewed with a strong focus on the literature from recent years. The action and physical-chemical behavior of hydrotropes are discussed in relation to co-solubilizers and surfactants. A definition of a hydrotrope is formulated, and it is demonstrated that the unique behavior of a hydrotrope, which distinguishes this class of substances from both co-solubilizers and regular surfactants, is that the aggregation is weak without a hydrophobic solute, but there is a pronounced reinforcement of aggregation in the presence of a hydrophobic solute.

The observations about this weak aggregation dating back to nearly a century, will be given together with most recent theory and establishment of microstructures involved, together with some applications in chemical engineering for efficient separation chemistry processes.

Reference:

Werner Kunz et al. : *Current Opinion in Colloid & Interface Science* 2016, **22**, 99–107

Notes :

Andreas Heuer

Institute of Physical Chemistry – Westfälische Wilhelms-Universität Münster, Germany

I. Non-linear driving of particles in disordered systems: a potential energy landscape perspective

The effect of driving particles in small external fields can be predicted via simple linear response theory. However, a priori it is not evident how the system behaves for large external fields. Different scenarios are discussed: (i) Driving a particle in a 3D disordered potential energy landscape (PEL). This scenario is, e.g., relevant for the non-linear conductivity of alkali ions in silicate systems. (ii) Driving a tagged particle in a supercooled liquid as achieved in microrheology. To better understand the resulting effects some key concepts of the PEL of glass-forming systems are introduced. The non-linear driving has some interesting consequences such as superdiffusive behavior, the emergence of effective temperatures to describe the non-linear mobility, or laning of the driven particles. Many of these observations can be rationalized in terms of properties of the PEL.

II. Shearing of glasses and supercooled liquids & Frame-guided assembly of amphiphilic molecules

In the main part of this talk I discuss results about the application of steady or oscillatory shear to glass-forming systems. One observes a specific stress response, resulting from local plastic events which are induced by the external shear. Here we show how this intricate interplay is determined by the potential energy landscape (PEL). The plastic events can, e.g., be related to the disappearance of saddles in the PEL upon shearing. Going beyond the previous analysis we show that even after many plastic events the system may possess a large memory concerning its initial unsheared configuration. This explains surprisingly strong memory effect in oscillatory shear experiments.

Furthermore, I briefly introduce a new concept to form micelles as introduced by the group of Dongsheng Liu (Tsinghua University, Beijing). Using a molecular frame it is possible to form micelles with specific shapes and radii. From the theoretical perspective we want to understand the additional driving force of frame-guided assembly as compared to the micelle formation without the frame. For this purpose we have defined a minimalistic model of amphiphilic molecules which allows us to model the micelle formation very efficiently. It turns out that significantly below the critical micellar concentration the presence of these frames enables the formation of well-defined micelles.

Notes :

Margarida Telo da Gama

Center for Theoretical and Computational Physics and Department of Physics, Faculty of Sciences – University of Lisbon, Portugal

I. Wetting of liquid crystals at structured substrates: statics and dynamics

Geometrically or chemically structured surfaces, on the scale of micrometers, are becoming increasingly available due to impressive developments of microfabrication techniques. The wetting properties of fluids on these surfaces received considerable attention owing to a wealth of new phenomena that includes surface phase transitions such as filling. When the fluid is ordered, as in nematics or cholesterics, the effects of elastic distortions on the mesoscale, and those of topological defects nucleated at or close the structured surfaces play a very important role, which will be discussed using theoretical tools (Frank-Oseen elasticity) and numerical techniques of appropriate mesoscopic (Landau-de Gennes) models.

References:

1. Complex fluids at complex surfaces: simply complicated? P Patrício, JM Romero-Enrique, NM Silvestre, NR Bernardino, MM Telo da Gama, *Molecular Physics* 109 (7-10), 1067-1075, 2011.
2. Nematic wetting and filling of crenellated surfaces, NM Silvestre, Z Eskandari, P Patrício, JM Romero-Enrique, MM Telo da Gama, *Physical Review E* 86 (1), 011703, 2012.
3. Interfacial motion in flexo- and order-electric switching between nematic filled states, ML Blow, MMT da Gama, *Journal of Physics: Condensed Matter* 25 (24), 245103, 2013.
4. Structure of the cholesteric–isotropic interface, NR Bernardino, MCF Pereira, NM Silvestre, MMT da Gama, *Soft matter* 10 (47), 9399-9402, 2014.
5. Wetting of cholesteric liquid crystals, NM Silvestre, MCF Pereira, NR Bernardino, MMT da Gama, *The European Physical Journal E* 39 (2), 1-6, 2016.

II. Nematic films at structured surfaces: anchoring transitions and elastic instabilities

Away from coexistence, liquid crystals at structured surfaces may exhibit anchoring transitions and static and dynamical instabilities. I will review recent results theoretical and numerical results, focused on the analysis, at the mesoscale, of the effects of elastic distortions and topological defects for nematic films on a variety of structured surfaces.

References:

1. Nematic films at chemically structured surfaces, NM Silvestre, MMT da Gama, M Tasinkevych, *Journal of Physics: Condensed Matter* 29 (7), 074002, 2017.
2. Pattern-induced anchoring transitions in nematic liquid crystals, O A Rojas-Gómez, JM Romero-Enrique, NM Silvestre, MMT da Gama, *Journal of Physics: Condensed Matter* 29 (6), 064002, 2016.
3. Nematic liquid crystals on sinusoidal channels: the zigzag instability, NM Silvestre, JM Romero-Enrique, MMT da Gama, *Journal of Physics: Condensed Matter* 29 (1), 014004, 2016.
4. Nematic droplets on fibers, VMO Batista, NM Silvestre, MMT da Gama, *Physical Review E* 92 (6), 062507, 2015.
5. The effect of anchoring on the nematic flow in channels, VMO Batista, ML Blow, MMT da Gama, *Soft matter* 11 (23), 4674-4685, 2015.

Notes :

Bradley D. Olsen

Dept. of Chemical Engineering – Massachusetts Institute of Technology, Cambridge, USA

I. Swelling and Mechanics of Polymer Networks

Transcending applications such as actuators, baby diapers, food, biomedical materials, and car tires, polymer networks are some of the most ubiquitous soft materials in use today. In most application, the use of these gels relies on their ability to swell with solvent and their mechanical response, properties that share a common origin in the entropic elasticity of polymer chains. This lecture will review the venerable theories for network properties, with a particular focus on developments in the theory of gel swelling and exploring the competing theories of gel elasticity.

II. Effect of Defects on the Properties of Polymer Networks

The design of polymer networks is one of the oldest and most important challenges in chemistry, impacting many of the highest volume chemical industries from rubber to adhesives to biomedical materials. However, more than any other branch of materials, networks have resisted precise characterization. This leaves many open challenges in understanding how their chemical design is linked to their physical properties of relevance for applications such as food science, biomedical materials, and consumer products. This lecture will discuss recent advances in our understanding of how defects in polymer networks affect their properties.

New theories for characterizing the topology and mechanics of chemical networks will be presented. Driven by advances in a collaborator's group that enable direct measurements of primary loops in polymer networks for the first time, we have been able to develop and validate parameter-free theories for predicting the kinetics of network formation, accounting for network defects. Using these theories, we can then develop a real elastic network theory built upon the classical phantom network theory that quantitatively accounts for network defects in calculating mechanical response. Rheological measurements confirm the validity of this theory, again with no variable parameters. These results are explored as a function of junction functionality, and the impact on gel point is also explored.

Notes :

Poster Sessions

Session 1

1	An Pham Duke University (Yellen)	Phase transition in two-dimensional colloidal suspension using rotating magnetic fields
2	Ankush Singhal MPIKG (Grafmüller)	Multiscale Modelling of Natural Polysaccharides
3	Davoud Mozhdehi Duke University (Chilkoti)	Genetically Encoded Lipid-Polypeptide Hybrid Biomaterials
4	Dong Wang Duke University (Behringer)	Origin of Shear Jamming for Frictional Grains
5	Yuxin Xie NC State (Yingling)	Comparison of Lower Critical Solution Temperature in Natural and Synthetic Macromolecules
6	Dishit Parekh NC State (Dickey)	Understanding & Controlling the Surface Wetting Phenomena of Ga-based Liquid Metals on Silicon-based Organic Polymers
7	Esra Oguztürk TU Berlin (Gradzielski)	Supraparticles Fabricated from Microfibrillated Cellulose
8	Jessica Nash NC State (Yingling)	Computational Design of Biomimetic Nanoparticles for Nucleic Acid Packaging
9	Jason Miles NC State (Genzer)	Design and Fabrication of Wettability and Chemical Gradients Through Degrafting
10	Jose Angel Danglad MPIKG (Riegler)	Quantitative Analysis of Polymer/Particle Mixtures in Ultrathin Films
11	Josua Grawitter TU Berlin (Stark)	Light-switchable molecules at planar fluid interfaces
12	Kohee Han NC State (Velev)	Magnetic Microbots and Microswimmers Based on Assemblies of Metallo-Dielectric Microcubes
13	Ryan Maloney NC State (Hall)	Computational Investigations of Two-Dimensional Systems of Colloids
14	Marek Sokolowski TU Berlin (Gradzielski)	Nanoparticle adsorption on supported lipid bilayers
15	Navarro, Luis Duke University (Zauscher)	Diblock Copolymers for Functional Surface Coatings

Session 2

16	Abdul Rauf HU Berlin (Rabe)	Quantitative Nanomechanical Mapping and Contact Mode Imaging of Graphene-mica Slitpore
17	Daniel Armstrong NC State (Spontak)	Shape Memory Thermoplastic Elastomers as Bimorph Electroactive Polymers
18	Francesco Bonazzi MPIKG (Weikl)	Interactions of membranes with nanoparticles and proteins: An elastic-membrane model
19	Eleanor Ewins MPIKG (Dimova)	Probing particle-membrane interactions using giant vesicles
20	Guo-Jun Liao TU berlin (Klapp)	Collective Phenomena of Spherical Circle Swimmers Dispersed on a Monolayer
21	Jacek Walkowiak HZ Berlin (Ballauff)	Interaction of spherical polyelectrolyte brushes with proteins
22	Jana Staffa TU Berlin (Hildebrandt)	Spectroscopic studies of electric fields at biomimetic interfaces
23	Kaihang Shi NC State (Gubbins)	Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface
24	Natasha Morales Castellanos NC State (Velev)	Nanocapillary binding as a tool in the assembly of novel responsive colloidal structures, patchy particle clusters and inks for 3D printing
25	Radhika Vaid NC State (Pasquinelli)	Determine degradation mechanism of bioresorbable polymers by integrating experiments and computational techniques
26	Stefanie Wandrei TU Berlin (Schoen)	The effect of polydispersity on the behavior of magnetic colloidal suspensions
27	Yiliang Lin NC State (Dickey/Genzer)	Liquid Metal Nanomaterials for Soft Electronics and Drug Delivery
28	Ting Ge UNC Chapel Hill (Rubinstein)	Nanoparticle Motion in Entangled Melts of Linear and Nonconcatenated Ring Polymers
29	Yangju Lin Duke University (Craig)	Correlating Single Molecule Mechanochemical Response with Macroscopic Mechanochromic Activity in a PDMS Elastomer

Round Table Discussions

Group A – Coray Colina/Martin Schoen (Thursday)

Josua Grawitter, Stefanie Wandrei, Daniel Armstrong, Jason Miles, Davoud Mozhdehi

1. Kyle E. Hart and Coray M. Colina: „Estimating gas permeability and permselectivity of microporous polymers”, *J. Membrane Sci.*, **468**, 259–268 (2014).
2. T. P. Liyana-Arachchi, J. F. Sturnfield, and C.M. Colina C.M, „Ultrathin Molecular-Layer-by-Layer Polyamide Membranes: Insights from Atomistic Molecular Simulations”, *J. Phys. Chem. B*, **120**, 9484–9494 (2016).

Group B – William Ducker/Jürgen P. Rabe (Friday)

Marek Sokolowski, Eleanor Ewins, An Pham, Jessica Nash, Ryan Maloney

1. D. J. Mastropietro and W. A. Ducker, “Forces between Hydrophobic Solids in Concentrated Aqueous Salt Solution”, *Phys. Rev. Lett.*, **108**, 106101 (2012).
2. M. Kargar, A. Prudenb and W. A. Ducker, “Preventing bacterial colonization using colloidal crystals”, *J. Mater. Chem. B*, **2**, 5962 (2014).

Group C – Thomas Zemb/Stefan Zauscher (Thursday)

Francesco Bonazzi, Abdul Rauf, Yangju Lin, Radhika Vaid

1. M. Kellermeier, A. Picker, A. Kempter, H Cölfen, and D. Gebauer, “A Straightforward Treatment of Activity in Aqueous CaCO₃ Solutions and the Consequences for Nucleation Theory”, *Adv. Mater.*, **26**, 752–757 (2014).
2. S. Schöttl and D. Horinek, “Aggregation in detergent-free ternary mixtures with microemulsion-like properties”, *Curr. Opin. Colloid Interface Sci.*, **22**, 8–13 (2016).

Group D – Bhuvnesh Bharti/Jan Genzer (Thursday)

Jose Angel Dangelad, Jana Staffa, Luis Navarro, Kaihang Shi, Dong Wang

1. B. Bharti, A.-L. Fameau, M. Rubinstein, and O. D. Velev, “Nanocapillarity-mediated magnetic assembly of nanoparticles into ultraflexible filaments and reconfigurable networks”, *Nature Mater.*, **14**, 1104–1109 (2015).
2. B. Bharti, D. Rutkowski, K. Han, A. U. Kumar, C. K. Hall, and O. D. Velev, “Capillary Bridging as a Tool for Assembling Discrete Clusters of Patchy Particles”, *J. Am. Chem. Soc.*, **138**, 14948–14953 (2016).

Group E – Andreas Heuer/Sabine Klapp (Friday)

Ankush Singhal, Jacek Walkowiak, Dishit Parekh, Yuxin Xie, Natasha Morales Castellanos

1. A. Heuer and L. Lühning, “Physical mechanisms of nonlinear conductivity: A model analysis”, *J. Chem. Phys.*, **140**, 094508 (2014).
2. C. F. E. Schroer and A. Heuer, “Anomalous Diffusion of Driven Particles in Supercooled Liquids”, *Phys. Rev. Lett.*, **110**, 067801 (2013).

Group F – Magarida Telo da Gama/Martin Schoen (Friday)

Esra Oguztürk, Guo-Jun Liao, Koohee Han, Yiliang Lin, Ting Ge

1. P. Patrício, J. M. Romero-Enrique, N. M. Silvestre, N. R. Bernardino, and M. M. Telo da Gama, “Complex fluids at complex surfaces: simply complicated?”, *Mol. Phys.*, **109**, 7–10, 1067–1075 (2011).
2. N. M. Silvestre, J. M. Romero-Enrique, and M. M. Telo da Gama, “Nematic liquid crystals on sinusoidal channels: the zigzag instability”, *J. Phys. Condens. Matter*, **29**, 014004 (2017).

Notes

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