Virginia Soft Matter Workshop IV

Virginia Commonwealth University

Oct. 29, 2016

9:00 AM – 9:10 AM	Welcome Remarks	
Session Chair – Dr. Christina Tang		
9:10 AM – 9:55 AM	**Dr. Orlin D. Velev – NC State University: "Dynamically Reconfigurable Soft Matter in External Fields"**	
10:00 AM – 10:30 AM **Soundbite Session I**	Ryan Grosenick	Self-assembly of Artificial Actin-like Filaments
	Justin Barone	Protein-polymer nanocomposites
	Christopher Dosier	Alginate Microbead Technology for Delivery of Biologics
	Ami Jo	Engineering Polymeric Nanoparticles for Diagnostics and Drug Delivery
	Assad Ullah Khan	Plasmonic Nanoparticles as Sensors to Probe Polymer Brush Formation
	Yow-Ren Chang	Hindering bacterial biofilm formation using surface topography
	Jiten Narang	Anisotropic Stiffness Micropillar Arrays Influence Cell Organization, Differentiation and Migration
	Zach Schuhmacher	Using PDMS to investigate the properties of Intrinsic Foot Muscles
	Shani Levit	Electrospinning to Extend Shelf-life and Stability of Nanomedicines
10:30 AM – 10:45 AM	*COFFEE BREAK*	
Session Chair – Dr. Hooman Tafreshi		
10:45 AM – 11:15 AM	**Dr. Alenka Luzar – VCU: "Molecular Modeling of Surface Wettability by External Stimuli"**	
11:15 AM – 11:45 AM	Michael K. Salerno	Coarse-Grained Polymer Models for Nanoscience Applications
	Weizhu Yang	A Novel Porous structure for enhanced Energy Absorption Performance
	Ralph Romero	Crumpling of an Elastic Ring in Two Dimensions

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Soundbite Session II	Yanfei Tang	Polyelectrolyte complexes in solution: a molecular dynamics study
	Yafei Wang	Numerical simulation of colloidal particle self-assembly in an evaporating micro-sized droplet
	Qingchang Liu	A Unified Mechanics Model of Wettability Gradient-Driven Motion of Water Droplet on Solid Surfaces
	Charles E Smith	Variable "time constants" for simple quantum systems
	Yuan Gao	Mechanically Tunable Thermal Conductivity in Bilayer Heterostructures
	Mahdi Shafiei	Dynamics of Water under Electric Field
Session Chair – Dr. Joseph Reiner		
11:45 AM – 12:15 PM	**Dr. Joseph Robertson – NIST: " An Anthrax Toxin Biosensor fabricated by integrating pore-forming proteins into electroanalytical interfaces"**	
12:15 PM – 1:00 PM	*LUNCH*	
Session Chair – Dr. Hong Zhao		
1:00 PM – 1:30 PM	**Dr. Weiwei Deng – Virginia Tech: "Reshape Liquid Jets, Droplets, and Particles with Electric Fields"**	
1:30 PM – 2:00 PM **Soundbite Session III**	Karam Almilaji	Superoleophobic Surfaces by Mask-assisted Electrospray
	Colin Qi	Solid Dispersion Lithium-Ion Flow Battery
	Zhengping Zhou	Controlling the Pore Size of Mesoporous Carbon Thin Films through Thermal and Solvent Annealing
	Hooman Tafreshi	Modeling Underwater Superhydrophobic Surfaces
	Geoffrey Geise	Polymer membrane research at U.Va.
	Mubashir Ansari	Dual Extrusion Technology for filament Fabrication used in Fused Deposition Modeling
	Maryanne Collinson	The Fabrication of Surface Chemical Gradients and the Importance of the Underlying Base Layer in Defining Gradient Wettability
	Prajakta Kamerkar	Influence of relative humidity on rheological characterizations of viscoelastic soft-solids

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2:00 PM – 2:30 PM	*COFFEE BREAK*	
Session Chair – Dr. Maryanne Collinson		
2:30 PM – 3:00 PM	**Dr. Kevin Caran – JMU: "Colloidal and Antibacterial Activity of Non-Conventional Amphiphiles"**	
3:00 PM – 3:45 PM **Soundbite Session IV**	Shengfeng Cheng	MACR program at Virginia Tech
	Sergei Egorov	Spin Relaxation in Organic Semiconductors
	Prudhvidhar Gaddam	A liquid state thermal diode (soundbite)
	William Morris	Quaternary Ammonium-Functionalized PPO Anion Exchange Materials With Variable Alkyl Side Chains
	Yuanyuan Ji	Specific Ion Effects in Charged Polymer Membranes
	Nan Yang	Studying Crystalline Morphology and Texture of Small Molecule Organic Semiconductor Thin Films
	Chester Szwejkowski	Pushing the Limits of Time Domain Thermo Reflectance with Soft Matter
	Joseph Reiner	Forensic applications of single cell and single molecule manipulation
	Yue Zhang	Liquid Evaporation-Driven Folding of Graphene with Surface wettability Gradients
3:45 PM – 4:00 PM	Wrap up	

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Dynamically Reconfigurable Soft Matter in External Fields: Smart Particle Gels, Engineered Clusters and Self-Propelling Microbots

Orlin D. Velev
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This talk will present strategies for electric and magnetic field driven assembly and manipulation of a rich variety of dynamic structures from soft matter. We have shown earlier how metallo-dielectric Janus/patchy spheres and microcubes acquire complex polarization patterns in external fields, leading to multidirectional interactions and assembly. Now we will first describe how magnetically responsive Janus microcubes can be assembled hierarchically into dynamically reconfiguring microclusters and chains. The residual polarization of the metal-coated facets leads to magnetic interactions and reconfiguration, directed by the orientational sequence of the microcubes in the chains. The pre-assembled clusters can be reversibly actuated, oriented and spatially transported by magnetic fields. They are capable of grabbing and transporting target micro-objects and serve as prototypes of new microbot and colloidal origami structures. They can also be designed to be self-motile in media with non-Newtonian rheology. In the second part of the talk, we will describe a new smart gel system of ultraflexible chains from magnetically responsive nanoparticles inside multiphase water-oil systems (*Nature Mater.* 14:1104 2015). The nanoparticles are coated by condensed, surface-anchored lipid shells. The field collects the super-paramagnetic nanoparticles into filaments by magnetophoresis, while the lipid shells form on contact nanocapillary liquid bridges between them. After switching off the field the particles retain their structural arrangement by a soft attractive potential induced by the liquid bridges. The nanocapillary binding allows for easy particle rolling and sliding and the resulting ultrahigh flexibility was measured to be orders of magnitude higher than other linear structures reported to date. The soft, "snappable," capillary interactions enable the making of magnetically self-repairing gel networks and novel inks for 3D printing.

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Molecular Modeling of Surface Wettability by External Stimuli

Alenka Luzar
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Molecular level understanding of the intelligent control of surface wettability by external stimuli can find real-world applications in nanofluidics and electro-optics. The talk will review our theoretical and molecular simulation works that predict and elucidate thermodynamic driving forces and kinetic factors pertinent to nanoconfined water. Examples will range from ordering of nanoparticles in dispersion, to nanoelectrowetting. A picture emerges in which molecular modeling can dissect nanoscale phenomena in ways that surprise. Applying this knowledge, we will show how to tailor wetting properties in a reversible manner, to make smart or responsive surfaces for dynamical tunable devices

An anthrax toxin biosensor fabricated by integrating pore-forming proteins into electroanalytical interfaces

Joseph W.F. Robertson, Vitalii Silin, Ariel Michelman-Ribero, Julianne S. Robbins, Kelby Peterson, Madeleine P. Gordon, Joseph E. Reiner, and John J. Kasianowicz
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The integration of complex biological molecules such as proteins with metal and semiconductor interfaces is limited by several inherent incompatibilities. To develop sensors based upon protein-protein interactions at such surfaces, three significant obstacles must be overcome: 1) the sensing protein must retain its native, or native-like structure, 2) the protein must be in electrical (or optical) contact with the metal surface and 3) the reporter protein much be at a sufficiently high concentration to produce a measurable, unambiguous signal. In this presentation, I will discuss the fabrication of polymer-tethered bilayer membranes, which provides a biomimetic interface capable of addressing each of the three obstacles. With inspiration taken from single molecule nanopore sensors, I will discuss the fabrication and characterization of an anthrax biosensor, and discuss strategies to optimize these sensors.

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Reshape liquid jets, droplets, and particles with electric fields

Weiwei Deng
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The electric field can play important roles in the breakup of liquid jets, deformation of droplets, and shaping micro/nano particles from drying of liquid solution. In this Talk, we begin with the breakup of liquid jets, which is ubiquitous with rich underpinning physics and widespread applications. The natural breakup of liquid jets originates from small ambient perturbations, which can grow exponentially until the amplitude as large as the jet radius is reached. For unelectrified jets, only the axisymmetric perturbation is possibly unstable, and this mode is referred as varicose instability. For electrified jets, the presence of surface charge enables additional unstable modes, among which the most common one is the whipping instability that bends and stretches the charged jet. I will report the interesting outcomes of breakup of electrified jets that undergo both varicose and whipping instabilities. The co-development of transverse and axisymmetric perturbations leads to remarkable jet breakup behavior attributable to initial perturbation magnitude, perturbation wavenumbers, and jet surface charge levels. The well-controlled triggering and co- development of the instabilities expands the possibilities of electrified jets breakup, and may spawn new ways of generating micro/nano droplets and controlled electrospinning. I will also show examples of creating non-spherical micro/nano particles with the aid of electric fields, and discuss two examples: non-spherical nanoparticles for cancer drug delivery, and fabrication of semi-organized semiconducting polymer nano pillars with superior charge mobilities.

Colloidal and Antibacterial Activity of Non-Conventional Amphiphiles

Kevin Caran
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Over the past 5 years, our research laboratory has prepared a number of novel surfactants with a variety of non-conventional structures. These include compounds with two to six polar cationic head groups and one to three non-polar tails. This work has allowed us to begin to develop an understanding of the relationship between amphiphile structure and colloidal activity, as measured by critical aggregation concentration in aqueous solution. Collaborations with JMU Biology and JMU Physics have also led to an understanding of the relationship between structure and antibacterial and foam-forming ability, respectively. This has led to the development of several compounds with high antibacterial activity. Ongoing work aims to optimize our search for potent and fast-acting antiseptics.