VT-ORNL Joint Symposium on Soft Matter and Biological Physics

Scientific Program

Wednesday, May 17, 2023 (Hahn Hall North Auditorium)

9:00 – 9:15 Opening speech by Prof. Kevin Pitts (COS Dean)
Opening speech by Prof. Randy Heflin (SVP for Research and Innovation)
Welcome speech by Prof. Mark Pitt (Physics Department Chair)
Welcome speech by Prof. Shengfeng Cheng (Director of CSMBP)

Session I: Chair TBD

9:15 – 10:00 *Keynote: Prof. Flora Meilleur* (ORNL and North Carolina State University)
Activation of molecular dioxygen by lytic polysaccharide monooxygenases

10:00 – 10:15 Jiangtao Cheng ( )
10:15 – 10:30 Bahareh Behkam ( )
10:30 – 10:45 Wenya Shu ( )

10:45 – 11:00 Coffee Break

Session II: Chair TBD

11:00 – 11:45 *Keynote: Prof. Mark Dadmun* (ORNL and University of Tennessee)
Correlating Structure of Functional Polymeric Systems to Performance with Neutron Scattering

11:45 – 12:00 Lou Madsen ( )
12:00 – 12:15 Michael Bartlett ( )
12:15 – 12:30 Guoliang Liu ( )

12:30 – 1:30 Lunch

Session III: Chair TBD

1:30 – 2:00 *Invited Talk: Yangyang Wang* (ORNL)
Spatial Correlations of Polymer Dynamics

2:00 – 2:15 Justin Barone ( )
2:15 – 2:30 Shengfeng Cheng ( )
2:30 – 3:00 *Invited Talk:* Jan-Michael Carrillo (ORNL)
Beyond Implicit Solvents: Advancing Soft Matter Simulations with Explicit Solvent Molecular Dynamics

3:00 – 3:15 Coffee Break

Session IV: Chair TBD

3:15 – 4:00 Keynote Speaker: Benjamin Doughty (ORNL)
Soft Matter Interfaces At and Away from Equilibrium

4:00 – 4:15 James McClure ( )
4:15 – 4:40 *Invited Talk:* John Katsaras (ORNL)
TBD

4:45 – 5:00 Rana Ashkar ( )

5:00 – 6:00 Coffee Break, Poster Session (Best Poster Award), Collaboration Proposal Competition

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Thursday, May 19, 2023 (Hahn Hall North130 & Auditorium)

8:30 – 8:40 Opening notes, Rana Ashkar

Session V: Chair TBD

8:40 – 9:40 *Dr. Benjamin Doughty*
Tutorial: An Introduction to Probing Surfaces with Nonlinear Optics

9:40 – 10:00 Coffee Break

Session VI: Chair TBD

10:00 – 11:00 *Prof. Mark Dadmun*
Tutorial: Tailor Made Polymeric Feedstocks for Additive Manufacturing Using Polymer Science Principles

11:00 – 11:20 Coffee Break

Session VII: Chair TBD

11:20 – 12:20 *Prof. Flora Meilleur*
Tutorial: Neutron crystallography to model hydrogen atoms in protein structures

12:30 – 2:30 Working Lunch and Round Table Discussion

2:30 Symposium concludes.

For virtual attendees, the Zoom meeting link is:

Meeting ID:
Passcode:

Abstracts of Keynote Talks

Prof. Flora Meilleur (ORNL and North Carolina State University)

Activation of molecular dioxygen by lytic polysaccharide monooxygenases.

Abstract: Lytic polysaccharide monooxygenases (LPMOs) are a unique class of mononuclear copper enzymes capable of oxidizing carbohydrates. LPMOs require the input of electrons and of O_2 or H_2O_2 to achieve hydroxylation of one carbon in the glycosidic bond. Despite extensive structural, biochemical and biophysical studies, the reaction mechanism remains elusive. We combine high resolution X-ray and neutron crystallography and computational simulations to investigate the activation of O_2 by LPMOs. Our structural studies aim to address outstanding questions on the role of second shell residues in the activation of O_2 and ultimately to determine the chemical nature of the intermediate responsible for hydrogen atom abstraction from the substrate. The ability to pinpoint hydrogen atoms to determine protonation states at and around the active site through the catalytic pathway is key to deciphering the chemistry catalyzed by LPMOs. Our experimental approach delivers precise, all atom structures that can reveal i) the positions and interactions of all hydrogen atoms in the enzyme, ii) atomistic details of the active site without perturbing the metal oxidation state, and iii) the chemical nature of the activated dioxygen species coordinated to the active site copper. I will present our recent neutron crystallographic studies that provide insights into the LPMO mechanism.

Prof. Mark Dadmun (ORNL and University of Tennessee)

Correlating Structure of Functional Polymeric Systems to Performance with Neutron Scattering

Abstract: Small angle scattering is often used to determine the size and shape of polymeric materials, but more thorough analysis of the scattering from multi-component polymer systems provides interfacial surface area, average domain size, and importantly, phase composition. For instance, polyimide aerogels (PIA) saturated with ionic liquids are promising materials as robust electrolytes for next generation batteries. Careful analysis of SANS data from PIA/ionic liquid constructs show that the ionic liquid penetrates the polyimide skeleton. This unexpected structure clearly impacts charge transport and therefore performance of the aerogel as a battery component. This mixing behavior must be more fully understood to rationally utilize these promising materials in devices. We will also present examples of how similar analyses of scattering data provide crucial insight into the correlation of thermodynamic structure and performance in novel soft electrolytes, 3D printed structures, and organic radical polymers.

Dr. Benjamin Doughty (ORNL)

Soft Matter Interfaces At and Away from Equilibrium

Abstract: Interfaces are the gatekeepers to function in a long list of applications, yet challenges in probing the interfacial monolayer at relevant scales limit our ability to rationally tune them using chemical and physical handles. Here we will describe our approach using nonlinear vibrational spectroscopy to access the mechanisms of self-assembly at buried liquid/liquid interfaces at and away from equilibrium. We will discuss the similarities and differences between small oligomeric amphiphiles, lipids, and extractants to reveal key design rules in tailoring interfaces.

Abstracts of Invited Talks

Dr. Yangyang Wang (ORNL)

Spatial correlations of polymer dynamics

Abstract: Inelastic scattering techniques and computer simulations provide important means to study the dynamics of polymeric materials via analyses of spatiotemporal correlations of density and concentration fluctuations. However, interpreting such dynamic correlations is often challenging, as the molecular motions of polymers encompass a wide range of time and length scales. In this talk, we outline a powerful and model-independent approach to polymer dynamics, which focuses on analyzing the spatial correlations of density fluctuations. This method is complementary to the traditional paradigm of time correlation analysis at discrete wave numbers. Applications of the proposed spatial correlation analysis will be discussed in the context of our recent studies of equilibrium dynamics of entangled polymers as well as Brownian motions of polymers under flow.

Dr. Jan-Michael Carrillo (ORNL)

Beyond Implicit Solvents: Advancing Soft Matter Simulations with Explicit Solvent Molecular Dynamics

Abstract: Performing simulations of soft matter systems, particularly molecular dynamics simulations, often involve coarse graining the system's description while preserving the particle nature of the model. Included in this approach is to implicitly model the solvent as random forces acting on the particles, such as using a Langevin thermostat in a NVT ensemble simulation. This method reduces computation cost and speeds up the evolution of large-scale structures or features of the model due to the more shallow energy barriers in the free energy landscape. However, in certain scenarios, explicitly modeling the solvent becomes necessary. For example, the inclusion of a polar solvent in the model allows for more accurate representation of these systems at higher concentrations where the assumptions of a continuum dielectric medium and screened hydrodynamics break down. This talk will present three soft matter systems where solvent was explicitly included in the model, including a polyelectrolyte in semi-dilute solutions exhibiting Zimm dynamics, charged star polymer surfactant assembling in an interface with dielectric mismatch, and a lipid bilayer with a zwitterionic lipid head in a dipolar solvent with added salts and applied oscillating electric field, causing a charge imbalance and the membrane to act as a capacitor.

Dr. John Katsaras (ORNL)

Lipid Bilayers as Platforms for Understanding the Brain and for the Development of Neuromorphic Computing

Abstract: Phospholipid bilayers can be described as capacitors whose capacitance per unit area (specific capacitance, Cm) is determined by the thickness of the membrane and its dielectric constant, independent of applied voltage. When exposed to a newly developed electrical “training” stimulation protocol, capacitive energy storage in lipid membranes was enhanced in the form of long-term potentiation (LTP), which enables biological learning and long-term memory (Scott et al., Proc. Natl. Acad. Sci. 119, e2212195119 (2022)). In today’s seminar, we will discuss how LTP can be produced from a membrane that is continuously pumped into a nonequilibrium steady state, altering its dielectric properties, and how model membranes can be used to understand the molecular basis of biological memory and inform the development of neuromorphic computing.

Tutorials Description

An Introduction to Probing Interfaces with Nonlinear Optic (Dr. Benjamin Doughty)
Here I will discuss fundamental aspects of probing interfaces with nonlinear vibrational spectroscopies. We will discuss what makes these measurements unique, address some key advantages of these methods in obtaining molecular scale information, and detail some limitations and challenges. We will highlight how these approaches are complementary to a variety of scattering and computational approaches, making them a powerful tool in the arsenal available to researchers studying complex soft matter interfaces.

Tailor Made Polymeric Feedstocks for Additive Manufacturing Using Polymer Science Principle (Prof. Mark Dadmun)
3-D printing of polymers has become an important manufacturing process in industry and among hobbyists. Limiting anisotropy and residual stress in the design of geometrically complex and 3D printed structures via material extrusion additive manufacturing (AM) remains a critical issue that hampers the widespread adoption of the technology. In this tutorial, I will introduce 3D printing/Additive Manufacturing, discuss advantages and limitations of the technology and discuss soft material science-based solutions to molecularly engineer new materials that are designed to tolerate the complex shear and thermal histories of the 3D printing process to create more robust and reproducible structures. The production of bespoke polymer feedstocks for AM also opens new avenues to more thoroughly study the fundamental science problems associated with additive manufacturing.

Neutron crystallography to model hydrogen atoms in protein structures (Prof. Flora Meilleur)
Neutron protein crystallography is a structural technique that permits the localization of hydrogen atoms, thereby providing important mechanistic details of protein function. The tutorial will introduce the workflow for neutron crystallography from crystal preparation, through data collection at the Spallation Neutron Source and at the High Flux Isotope Reactor, to structure refinement and analysis of the neutron scattering length density maps. The complementarity of x-ray and neutron crystallography will be discussed.

List of Posters

Will be published soon!