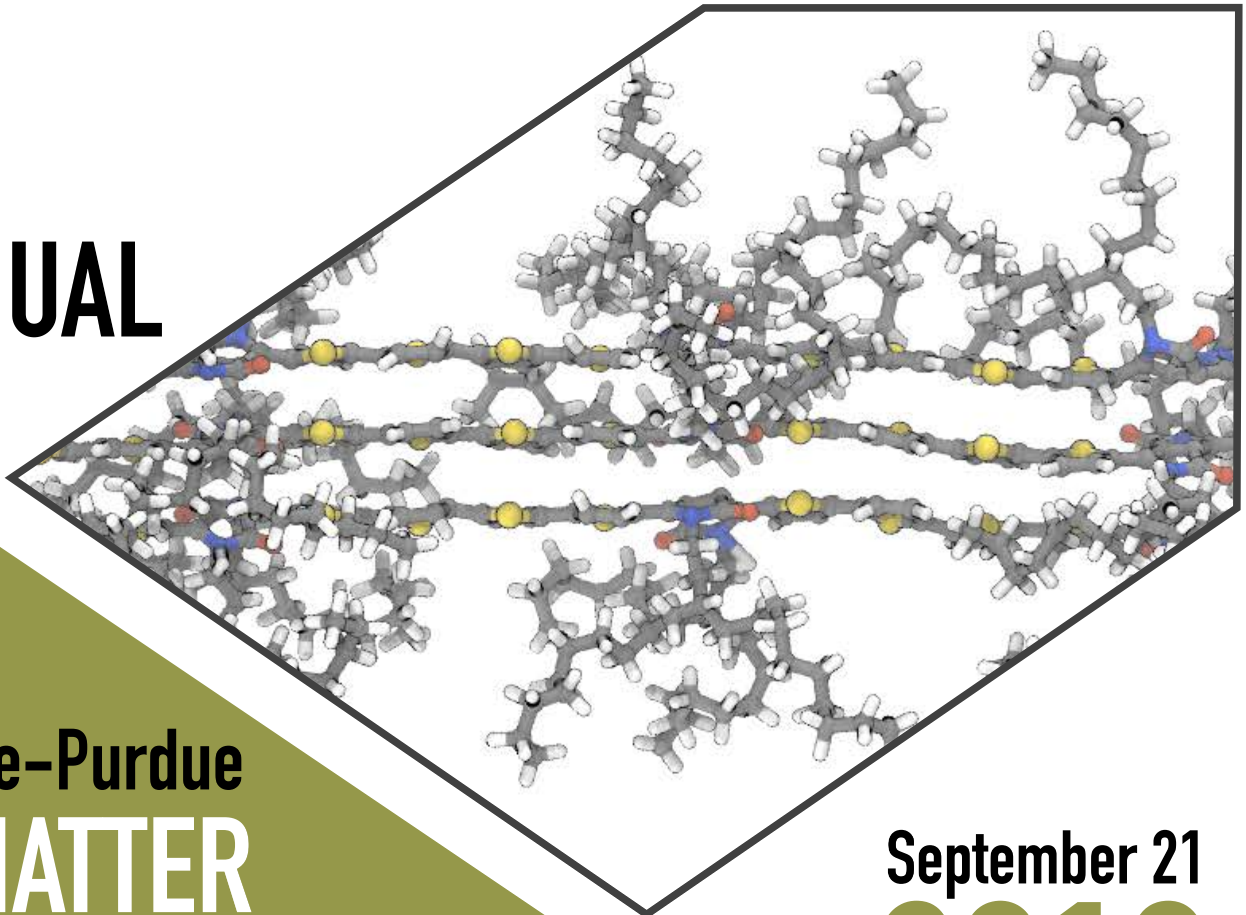
6TH ANNUAL



Notre Dame–Purdue

SOFT MATTER & POLYMERS SYMPOSIUM

September 21
2019

UNIVERSITY OF NOTRE DAME

Wilmeth Active Learning Center
Purdue University

PURDUE UNIVERSITY

Notre Dame-Purdue Symposium on Soft Matter & Polymers

Saturday, September 21st • Wilmeth Active Learning Center, Room 3087, Purdue University

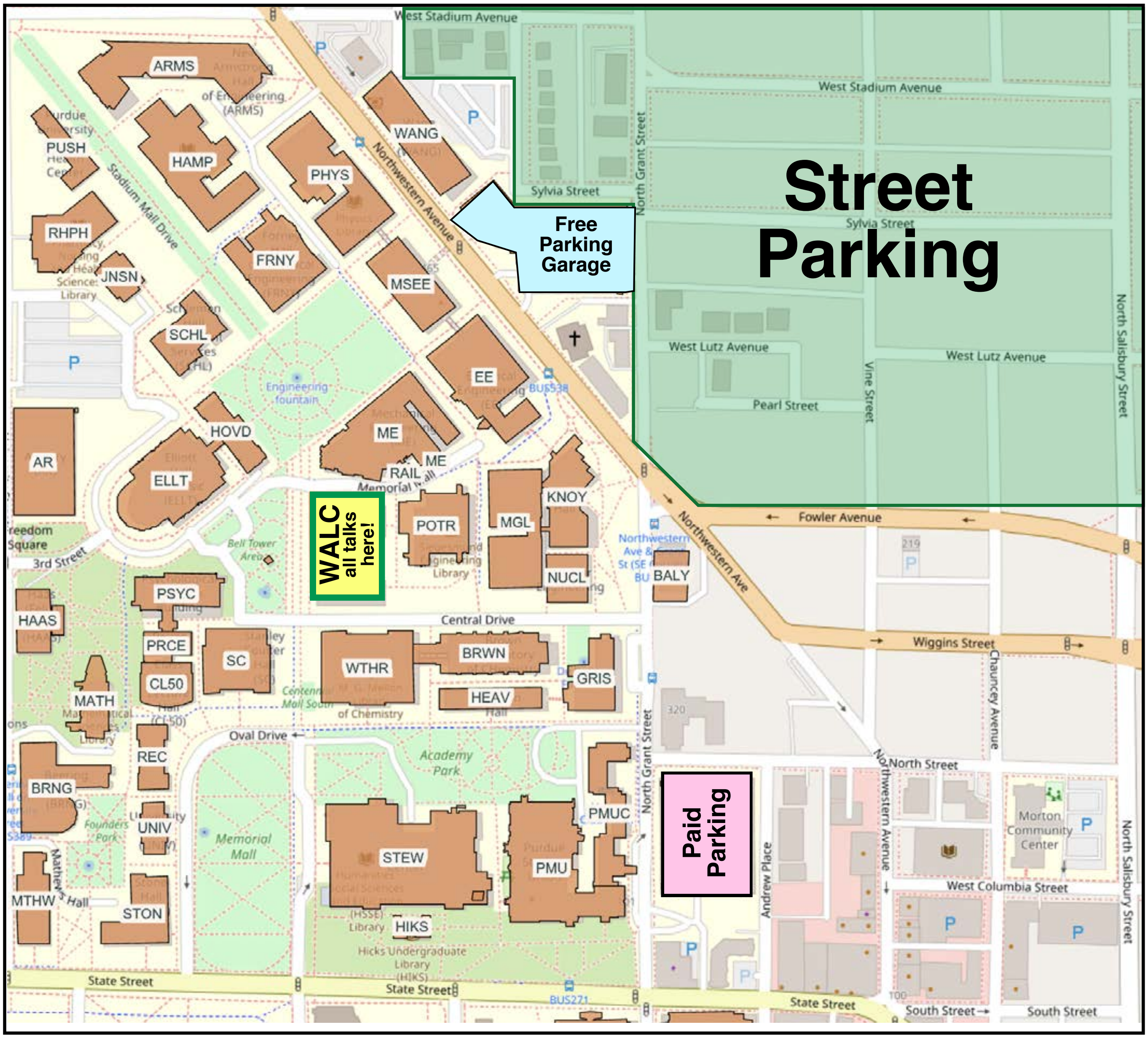
Organizers: Brett Savoie (bsavoie@purdue.edu), Matthew Webber (mwebber@nd.edu), Jianguo Mei (jgmei@purdue.edu), Haifeng Gao (hgao@nd.edu)

Registration Link: https://forms.gle/UN4nuo7mqkftnYfUA

8:30am	Breakfast and Check-in (Wilmeth Active Learning Center, Outside of Room 3087)	
	Technical Session 1 • Brett Savoie (chair)	
	Presenter	*Title*
9:20 am	Jonathan Wilker, Purdue University *Chemistry*	Adhesives at the Beach: Characterizing and Mimicking Biological Materials
9:40 am	Joona Bang, Korea University *Chemical and Biological Engineering*	Chemically and Thermally Stable Quantum Dots Prepared by Shell Encapsulation with Cross-linkable Polymer Ligands
10:00 am	Matthew Webber, Notre Dame *Chemical and Biomolecular Engineering*	Host-Guest Recognition for Functional Supramolecular Soft Materials
10:20 am	Coffee Break	
10:40 am	Vivek Narsimhan, Purdue University *Chemical Engineering*	Fluid mechanic studies of droplets with complex interfaces with applications to biology
11:00 am	Ruilan Guo, Notre Dame *Chemical and Biomolecular Engineering*	Hierarchically Functional Polymers for Advanced Membrane Separation Applications
11:20 am	Pedro E. Ramirez Gonzalez, UASLP, *Institute of Physics*	General Framework for the Study of Dynamical Properties and Arrested States of Ionic Liquids
11:40 am	Lunch, Wilmeth Active Learning Center (provided)	
	Technical Session 2 • Matthew Webber (chair)	
	Presenter	*Title*
1:20 pm	Ken Schweizer, University of Illinois *Materials Science and Engineering*	Glassy Dynamics, Kinetic Arrest and Transport in Colloidal, Molecular and Polymeric Liquids
2:00 pm	Jonathan Whitmer, Notre Dame *Chemical and Biomolecular Engineering*	Measuring the Driving Forces for Self Assembly
2:20 pm	Jim Caruthers, Purdue University *Chemical Engineering*	A model for describing the Arrhenian and super-Arrhenian behavior in glass forming small molecules and polymers
2:40 pm	Photo (WALC staircase) and poster setup (WALC, Room 3084/3087)	
3:20 pm	Chelsea Davis, Purdue University *Materials Engineering*	Illuminating interfacial mechanics: Coupling microscopy and mechanical testing to understand soft interfaces
3:40 pm	Jennifer Schaefer, Notre Dame *Chemical and Biomolecular Engineering*	Nanostructured Single-Ion Conducting Polymer Electrolytes
4:00-5:30pm	Poster Session (WALC, Room 3084/3087)	

Sponsors

Davidson School of Chemical Engineering



The symposium is being held in the Wilmeth Active Learning Center (WALC) in room 3087

The Northwestern parking garage is free (blue on map)

The Grant street parking garage costs money (red on map)

There is also free street parking in the neighborhoods northeast of campus

Symposium Abstracts

Jonathan Wilker

Purdue University
Chemistry

Adhesives at the Beach: Characterizing and Mimicking Biological Materials

Have you ever tried to use a glue and stick together anything when the substrates were wet? It probably didn't work. Yet take a look at sea creatures like mussels, barnacles, and oysters. How do they stick to the rocks- when living underwater? Our lab is working to understand how shellfish make adhesives for affixing themselves to surfaces. We are, then, using these insights to create biomimetic adhesive polymers. In doing so we have generated new materials that can bond more than Super Glue and also one of the strongest underwater adhesives seen. Applications for these new materials range from creating sustainable packaging to biomedical joining of tissues.

Joona Bang,

Korea University,
Chemical and
Biological Engineering

Chemically and Thermally Stable Quantum Dots Prepared by Shell Encapsulation with Cross-linkable Polymer Ligands

Endowing quantum dots (QDs) with robustness and durability has been one of the most important issues in this field, since the major limitations of QDs in practical applications are their thermal and oxidative instabilities. In this work, we propose a facile and effective passivation method to enhance the photochemical stability of QDs using polymeric double shell structures from thiol-terminated poly(methyl methacrylate-*b*-glycidyl methacrylate) (P(MMA-*b*-GMA)-SH) block copolymer ligands. To generate densely cross-linked network, the cross-linking reaction of GMA epoxides in PGMA block was conducted using Lewis acid catalyst under an ambient environment in order not to affect the photophysical properties of pristine QDs. This provides QDs encapsulated with robust double layers consisting of highly transparent PMMA outer-brush and oxidation-protective crosslinked inner-shell. Consequently, the resulting QDs exhibited exceptional tolerance to heat and oxidants when dispersed in organic solvents or QD-nanocomposite films, as evidently corroborated under various harsh conditions with respect to temperature and oxidant species. The present approach not only provides simple yet effective chemical means to enhance the thermochemical stability of QDs, but also offers a promising platform for the hybridization of QDs with polymeric materials for developing robust light-emitting or light-harvesting devices.

Matthew Webber,

University of Notre Dame,
Chemical and
Biomolecular Engineering

Host-Guest Recognition for Functional Supramolecular Soft Materials

Host–guest supramolecular recognition affords a useful tool in the physical crosslinking of macromeric precursors to create new hydrogel biomaterials with dynamic and controllable properties. In this work, we have probed the parameter of host–guest affinity in the design of hydrogel biomaterials of this class. The affinity of these interactions affords a molecular-scale approach to controlling the bulk dynamics of the material, which translates to tunable release of macromolecular payloads and dictates the rate of immune cell infiltration and material clearance in vivo. We subsequently couple host–guest affinity with thermally responsive macromers, affording two independent means to create injectable biomaterials. In building on these responsive soft materials, photo-responsive guest chemistries are also explored for external control of the affinity and dynamics of supramolecular recognition. The use of host–guest chemistry to create new biomaterials therefore affords precise and stimuli-responsive control of their bulk properties, serving to enhance the functionality of these systems in a variety of biological applications.

Vivek Narsimhan,
Purdue University,
Chemical Engineering

Fluid mechanic studies of droplets with complex interfaces with applications to biology

There is a lot of interest in characterizing the mechanics of complex interfaces that compose biological systems such as cells. In this talk, we discuss some of our recent work on the micromechanics of vesicles, i.e., sacs of fluid of ~20 microns containing a phospholipid bilayer. Here, we focus on how these systems behave in extensional flows, probing the conditions under which they become mechanically unstable and break up. We find that vesicles exhibit qualitatively different shape transitions than droplets under flow due to the bending and dilatational resistance of the phospholipid bilayer. We discuss the microfluidic experiments and boundary element simulations to quantify the different shape transitions, and describe how flow type and flow history alters these dynamics. In the second half of the talk, we discuss more general problems on how shear and dilatational resistance of a membrane alter the dynamics of droplet-like systems found in biology. We develop analytical theories to quantify how linear shear and dilatational surface moduli alter droplet translation, shape, breakup, and particle lift. We find that one can use simple scaling arguments to illuminate how interfacial moduli alter the translational speed a droplet.

Ruilan Guo,
University of Notre Dame,
Chemical and
Biomolecular Engineering

Hierarchically Functional Polymers for Advanced Membrane Separation Applications

Hierarchically functional polymer membranes with good chemical, mechanical, and thermal stability in the process environment are highly needed in many emerging energy and environment technologies, ranging from gas separation (e.g., carbon capture), water purification (e.g., desalination), to clean energy production (e.g., fuel cell). This presentation will describe new strategies for molecularly engineered polymer membranes that are both structurally and functionally rich for energy-efficient gas separations. An emphasis will be placed on most recent efforts based on iptycene-containing structural motif: microporous polymers with heterocyclic rings and ladder polymers with configurational free volume. The rich structural hierarchy and chemistry versatility of iptycene units offer great opportunities for generating well-defined yet highly tailorable microstructures and introducing unique supramolecular interactions which synergistically lead to intriguing membrane properties and exciting separation performance. Discussions will emphasize on the fundamental understanding and molecular design of modular structure-property relationships within this class of new polymer membranes.

Pedro E. Ramirez Gonzalez,
Autonomous University of
San Luis Potosi,
Institute of Physics

General Framework for the Study of Dynamical Properties and Arrested States of Ionic Liquids

In this work we present a first-principles theoretical framework for the description of structural and dynamical behavior in ionic liquids. This framework applies the recently developed Self-Consistent Generalized Langevin Equation (SCGLE) theory, which predicts the dynamically arrested states of such kinds of systems. As such, it is a particularly useful framework for predictions of arrested and partially arrested states in molten salts, electrolytic solutions, ionic superconductors, and room-temperature molten salts. Our framework has potential applications in the design and development of novel conducting material.

Ken Schweizer,
University of Illinois, Materials Science and Engineering

Glassy Dynamics, Kinetic Arrest and Transport in Colloidal, Molecular and Polymeric Liquids (**Keynote**)

Fundamental understanding of the spectacular slowing down of diffusion and structural relaxation in diverse classes of glass-forming liquids over 14 or more decades in time remains a scientific grand challenge. Moreover, glassy dynamics is relevant to key properties of functional polymeric materials such as nanocomposites, ion and electron conductors, separation membranes, and thermoplastics. I will present an overview of our work the last 5 years that has developed a microscopic, force-level, predictive statistical mechanical theory for activated relaxation, self-diffusion and elastic modulus. It addresses in a unified framework colloidal, molecular and polymeric liquids over the entire experimental range of relevant temperatures, densities and relaxation times. The fundamental structural relaxation event is of a mixed local-nonlocal character involving large amplitude barrier hopping on the cage scale that is strongly coupled to a longer range collective elastic fluctuation of the surrounding medium. Chemical complexity is treated in an a priori manner based on a physically motivated coarse graining procedure that exactly encodes the dimensionless compressibility (long wavelength density fluctuation amplitude) of real thermal liquids in a simplified model. Time permitting, generalization to the technologically important problem of activated penetrant diffusion in cold polymer melts and quenched glasses will be briefly discussed. Quantitative confrontation with experimental measurements will be presented throughout the talk.

Jonathan Whitmer,
University of Notre Dame, Chemical and Biomolecular Engineering

Measuring the Driving Forces for Self Assembly

Self-assembling systems, from the single-molecule to colloidal scales, may be controlled by learning the free energy landscapes controlling aggregation and growth. These may be extracted from molecular simulations using advanced sampling techniques derived from expanded-ensemble statistical mechanics. I will describe recent efforts by the Whitmer group to compute the free energy of assembly in two systems: host-guest macromolecular complexes and colloidal clusters. In the first case, the adaptive biasing force method is shown to obtain highly accurate estimates of the binding free energy, providing a path for future molecular engineering incorporating free energy calculations. In the second, we again use the adaptive biasing force algorithm to demonstrate a unique, particle-size dependent morphology transition in colloidal clusters and discuss how this might be used to engineer bespoke particle assemblies.

Jim Caruthers,
Purdue University, Chemical Engineering

A model for describing the Arrhenian and super-Arrhenian behavior in glass forming small molecules and polymers

In the liquid state small molecules and polymers exhibit a dramatic decrease in mobility of up to ten orders-of-magnitude as the temperature approaches the glass transition temperature Tg. This slow-down exhibits a super-Arrhenian temperature dependence that is perhaps the key signature of the glass transition – one of the major challenges in condensed matter physic. Using experimental data, it was shown that for 21 molecular glass formers a simple one-parameter model based on the excess internal energy accurately describes the super-Arrhenian behavior, whereas the well-known configurational entropy model of Adam-Gibbs shows significant deviations.[1] Also, it has been shown that excess internal energy model also describes the super-Arrhenian behavior of 12 polymeric glass formers.[2] Molecular dynamic simulations for the small molecule glass former ortho-terphenyl have recently been completed that quantitatively agree with experimental mobility data. The combined experimental and MD simulations span 16 orders-of-magnitude of mobility from the super-heated liquid at 100K above the boiling point to when the material falls out of equilibrium at Tg and includes pressures up through 2 GPa – this is the most extensive characterization of the mobility for any glass forming material. For all of these condition the mobility of orth-terphenyl is described the excess internal energy model.

[1] Caruthers and Medvedev, Phys. Rev. Mat. **2**, 055604 (2018)
[2] Medvedev and Caruthers, Macromol. **52**, 1424-1439 (2019)

Chelsea Davis,
Purdue University, Materials Engineering

Illuminating interfacial mechanics: Coupling microscopy and mechanical testing to understand soft interfaces

Many properties of polymeric systems are determined almost exclusively by the interfaces between various material components. This work focuses on various polymer interfaces and strategies to characterize their contact formation and debonding behavior. First, we utilize a mechanically-activated dye molecule covalently bound across the interface of a fiber-reinforced polymer composite (FRPC) to highlight interfacial stress transfer and debonding. The goal here was to develop a straightforward technique derived from commercially available materials that allows characterization of an FRPC interface by *in situ* mechanical deformation of single fiber model composites. Next, instrumented scratch experiments were performed on mechanophore-containing thermoset epoxy films to calibrate and quantify the fluorescence activation response of our mechanophore. This *in situ* mechanophore/mechanical deformation approach allows a diffraction-limited optical microscope to probe nanoscopic interfacial features in a powerful new way.

Finally, recent experiments highlighting the use of thin film buckling mechanics to characterize glassy film adhesion and Young's modulus will be presented. We utilize buckling instabilities as a novel way to measure thin glassy film delamination from soft substrates. Quantifying the strength of a particular film-substrate interface is challenging due to the brittleness of glassy films which can greatly complicate sample preparation, handling, and testing. Here, a method for measuring the adhesion of glassy thin films to soft elastomeric substrates is explored that exploits an understanding of surface buckling instabilities, specifically the transition from wrinkling to delamination (W2D). The adhesion (given by the critical strain energy release rate (G_c)) for two model materials interfaces is quantified by determining the critical delamination strain for two different polymer thin films (polystyrene (PS) and poly(methyl methacrylate) (PMMA)) and an elastomeric substrate (poly(dimethyl siloxane) (PDMS)). The G_c values determined for the PS-PDMS and PMMA-PDMS systems by W2D transition are 0.029 ± 0.01 J/m^2 and 0.025 ± 0.01 J/m^2, respectively. Overall, our work enables the development of new techniques to probe soft interfaces and deepen our understanding of polymer mechanics, reversible adhesion, and separation mechanisms.

Jennifer Schaefer,
University of Notre Dame, Chemical and Biomolecular Engineering

Nanostructured Single-Ion Conducting Polymer Electrolytes

Solvent-free polymer electrolytes have long been sought after for use in rechargeable batteries. The ideal electrolyte would have high ionic conductivity, a high active ion transference number, a wide electrochemical stability window, and chemical stability with the electrodes of interest. Poly(ethylene oxide)-based electrolytes have historically received the most research attention despite cation conduction rates being highly dependent on chain segmental motion. This talk will discuss the group's research on non-polyether, cation conducting, polyanion-based electrolytes. Single-ion conducting, side-chain polymer electrolytes are investigated wherein lithium conduction occurs in ionic domains or aggregates. The effect of polymer design and tethered anion chemistry on lithium transport will be discussed. In addition, we introduce novel multivalent cation conducting polymer electrolytes based on polyanions.

#	Poster Title and Authors
1	"Hierarchical Noncovalent Microcontact Printing of Striped Phase Lipids for Complex Ligand Presentation" Jeremiah Bechtold, Tyson Davis, Tyler Hayes, Terry Villarreal, and Shelley Claridge
2	"Investigating CB/SERS Detector Capabilities as a Function of Cucurbit[7]uril Macrocycle Geometry on Nanoparticle Surface" Adam S. Braegelman, Leonhard Karger, Lei Zou, Jon P. Camden, and Matthew J. Webber
3	"TBD" Saadia Chaudhry and Jianguo Mei*
4	"Influence of Residual Impurities on ROMP after CuAAC Click Chemistry" Jinwoong Choi, Jaewan Ko, Yoon Huh, Jeunggon Kim, and Joona Bang
5	"Accurate Determinations of Equilibrium Surface and Interfacial Tensions from Dynamic Values" Jaeyub Chung, An-Hsuan Hsieh, David S. Corti, Bryan W. Boudouris, and Elias I. Franses
6	"Intrinsically Microporous Pentiptycene-based Polymers for Enhanced Gas Separation Performance and Physical Aging Resistance" Tanner Corrado and Ruilan Guo
7	"Synthesis of Multisegmented Block Copolymers by Friedel-Crafts Hydroxyalkylation" Timothy Cuneo, Xiaosong Cao, Lei Zou and Haifeng Gao
8	"Utilizing the metal-mediated assembly of coiled-coil peptides to incorporate his-tagged cargo into designed, three-dimensional peptide crystals" Ryan W. Curtis, Manish Nepal, Michael J. Sheedlo, Chittaranjan Das, and Jean Chmielewski
9	"Adhesive Contact on an Unconfined Stretched Elastic Substrate" Naomi Deneke, Elina Ghimire, and Chelsea Davis
10	"Synthesis and photopatterning of norbornene modified hyaluronic acid" Fei Fan, Junyu Zhao, Laura Alderfer, and Donny Hanjaya-Putra
11	"Gel Polymer Electrolytes for Metal-Sulfur Batteries: Effect of Crosslinker Repeat Chemistry on Polysulfide Interactions" Hunter Ford, Jizhou Jiang, Peng He, and Jennifer Schaefer
12	"Highly Stable Lead-Free Perovskite Field Effect Transistors Incorporating Linear π-Conjugated Organic Ligands" Yao Gao and Letian Dou
13	"Controlling the Design of Multi-Functional Copolymer Nanofiltration Membranes" John R. Hoffman, Andrew Mikes, and William A. Phillip
14	"Microporous Polymeric Membranes for Gas Separations" Zihan Huang and Ruilan Guo
15	"Surveying the Free Energy Landscape of Clusters of Attractive Colloidal Spheres" Shanghui Huang, Michael Quevillon, Soren Kyhl, and Jonathan K. Whitmer
16	"Transfer Learning: Applications in Chemistry and Chemical Engineering" Nicolae Iovanac and Brett M. Savoie
17	"Introducing Negatively Charged Phosphorus Groups into DOPA containing Biomimetic Polymer Mimics" Taylor Jones and Jonathan Wilker
18	"Reversible Hierarchical Assembly of a Trimeric Coiled-Coil Peptide for Cell Encapsulation" Michael Jorgensen and Jean Chmielewski
19	"Simplified Molecular Dynamics Model for Mixed Conducting Polymers" Aditi Khot and Brett M. Savoie
20	"Highly Permeable and Selective Crosslinked Pentiptycene-based Polymer Membranes for Gas Separation" Si Li and Ruilan Guo

#	Poster Title and Authors
21	"The Effect of Humidity on the performance of the CsPbI3 perovskite solar cells" Haimin Li and Letian Dou
22	"Non-solvating, side-chain polymer electrolytes as lithium single-ion conductors: synthesis and ion transport characterization" Jiacheng Liu, Bumjun Park, Sunil P. Upadhyay, and Jennifer L. Schaefer
23	"Lactone-Substituted Isoindigo as a Simple and Strong Acceptor for Conjugated Polymers" Xuyi Luo, Dung T. Tran, and Jianguo Mei
24	"Cellulose Nanocrystal Coated Polymer Films-The Next Generation of Sustainable High Barrier Packaging Film" Md Nuruddin, Reaz A. Chowdhury, Jeffrey Youngblood, and John Howarter
25	"Magnesium ion conduction in dual cation exchanged poly(ionic liquid)s electrolytes" Bumjun Park, Hunter Ford, Laura Merrill, Jiacheng Liu, Loyal Murphy, and Jennifer Schaefer
26	"Amide side-chains enabling aqueous electrolyte compatibility in conjugated polymers" Kuluni Perera, Zhengran Yi, Liyan You, Zhifan Ke and Jianguo Mei
27	"Designing adhesives for different applications using biomimetic materials" Amelia A. Putnam and Jonathan J. Wilker
28	"Nanocellulose Film Modulus Determination Using Buckling Mechanics Approaches" Mitchell L. Rencheck, Ricardo Rodriguez, Nolan A. Miller, Drew Weiss, Sami M. El Awad Azrak, Endrina Forti, Md. Nuruddin, Jeffrey Youngblood, and Chelsea S. Davis
29	"Universal Engineering of Small Organic Dyes into Fluorescent Crystals by Hierarchical Assembly" Christopher R. Benson, Laura Kacenauskaite, Katherine L. VanDenburgh, Wei Zhao, Bo Qiao, Tumpa Sadhukhan, Maren Pink, Junsheng Chen, Sina Borgi, Chun-Hsing Chen, Krishnan Raghavachari, Bo W. Laursen and Amar H Flood
30	"Novel Elastic Response in Twist-Bend Nematic Models" Jiale Shi, Hythem Sidky, and Jonathan K. Whitmer
31	"Surface Cation Substitution-Effects on 2-D Perovskite Stability and Optoelectronic Properties" Stephen Shiring and Brett M. Savoie
32	"polymer thin film adhesion on soft elastic substrate through buckling delamination" Hyeyoung Son, Allison Chau, and Chelsea Davis
33	"Transport Inside Nitroxide-Based Radicals" Ying Tan, Bryan W. Boudouris, and Brett M. Savoie
34	"Effects of Side Chain on High Temperature Operation Stability of Conjugated Polymers" Dung T. Tran, Aristide Gumyusenge, Xuyi Luo, Zhengran Yi, Michael Roders, Alexander L. Ayzner, and Jianguo Mei
35	"High free volume ionic polymers for water desalination applications" Tao Wang, Feng Gao, and Ruilan Guo
36	"Synthesis and application of hyperbranched polyelectrolytes" Hui Xu, Xiaosong Cao, Weiping gan, Timothy Cuneo, and Haifeng Gao
37	"Excess Internal Energy Model for Super-Arrhenian Relaxation Dynamics of Super-Cooled Liquids" Jack Yungbluth and Brett M. Savoie
38	"Enthalpy of Formation Prediction via TAFFI Group Increment Theory" Qiyuan Zhao and Brett M. Savoie
39	"Dual-Responsive Supramolecular Hydrogels via Cucurbit[8]uril Ternary Complex Formation" Lei Zou and Matthew Webber