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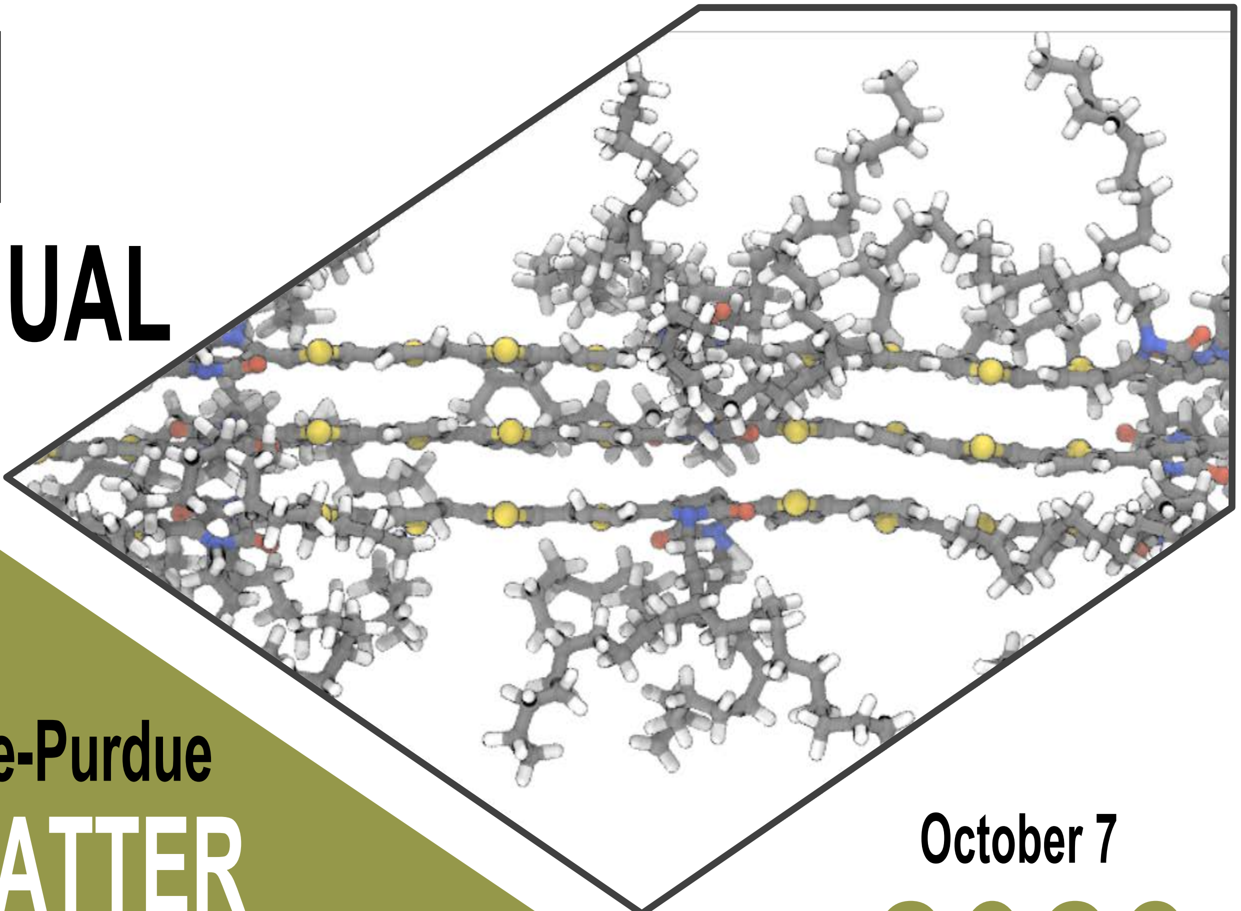

Notre Dame-Purdue

SOFT MATTER & POLYMERS SYMPOSIUM

October 7

2023

UNIVERSITY OF NOTRE DAME

Wilmeth Active Learning Center

PURDUE UNIVERSITY

Purdue University

Notre Dame-Purdue Symposium on Soft Matter & Polymers

Saturday, October 7, 2023 • Wilmeth Active Learning Center, Room 2087

Organizers: Letian Dou (dou10@purdue.edu), Jianguo Mei (jgmei@purdue.edu), Brett Savoie (bsavoie@purdue.edu), Matthew Webber (mwebber@nd.edu), Yichun Wang (ywang65@nd.edu)

Registration Link: Click Here to Register.

8:30 am	Breakfast and Check-in (Wilmeth Active Learning Center, Rm 2088)	
9:10 am	**Technical Session 1 • Letian Dou (chair)**	
	Presenter	*Title*
9:20 am	Brett Savoie, Purdue University *Chemical Engineering*	Is Predictive Materials Degradation Within Reach?
9:50 am	Gabriel Burks, University of Notre Dame *Chemical and Biomolecular Engineering*	Exploring the Nanoscale: In-situ TEM and Multimodal Characterization of Soft Matter
10:20 am	Coffee Break	
10:30 am	Yiying Wu, Ohio State University *Chemistry and Biochemistry*	Organic-Inorganic Lead Iodide: from Machine Learning to Materials Design
11:10 am	Shelley Claridge, Purdue University *Chemistry and Biomedical Engineering*	Plenty of Room at the Top: Hierarchical Chemical Patterning of Soft Materials
11:40 am	Lunch, Wilmeth Active Learning Center (provided)	
1:00 pm	**Technical Session 2 • Yichun Wang (chair)**	
	Presenter	*Title*
1:00 pm	Meenal Datta, University of Notre Dame *Aerospace and Mechanical Engineering*	Abnormal Mechanics in Brain Tumors: Implications for Hydrogel-Based Models
1:30 pm	You-Yeon Won, Purdue University *Chemical Engineering*	Advancing a Novel Polymer Lung Surfactant (PLS) Therapy for ARDS Treatment through Polymer Physics Research
2:00 pm	Tengfei Luo, University of Notre Dame *Aerospace and Mechanical Engineering*	A model for describing the Arrhenian and super-Arrhenian behavior in glass forming small molecules and polymers
2:30 pm	Short break and poster setup (WALC, Room 2088/2124)	
2:50 pm	Jonathan Whitmer, University of Notre Dame *Chemical and Biomolecular Engineering*	Entropy-enhanced Phase Separation in Polyelectrolyte Solutions
3:20 pm	Alexander Wei, Purdue University *Chemistry and Materials Engineering*	Tunable Rigidochromism of Copper–Pyrazolate Complexes
4:00-5:30pm	Poster Session (WALC, Room 2088/2124)	
5:45 pm	Best posters announced	

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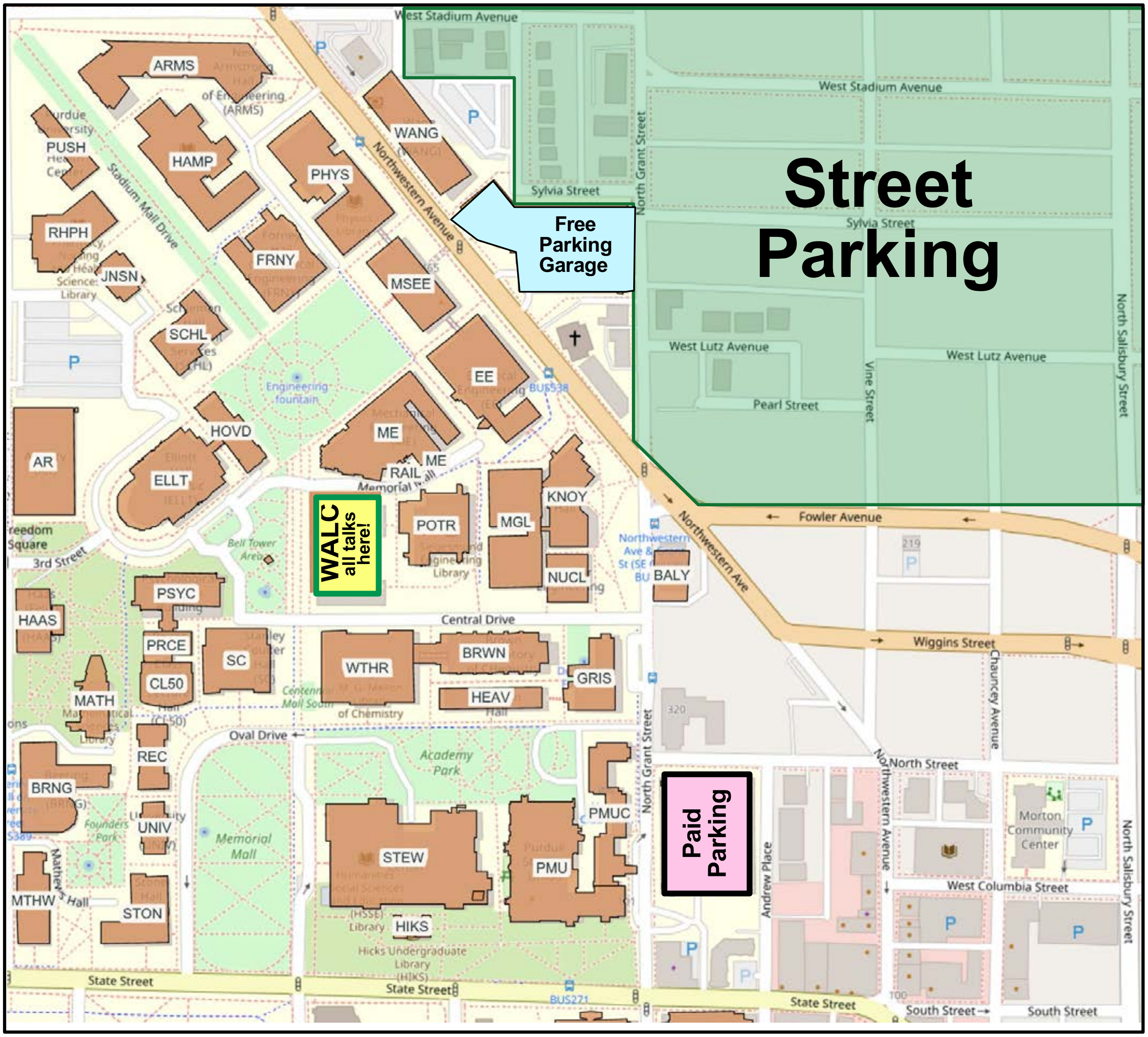

The symposium is being held in the Wilmeth Active Learning Center (WALC) in room 2087

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

Brett Savoie
Purdue University
Chemical Engineering

Is Predictive Materials Degradation Within Reach?

Limited stability and unacceptable degradation products are common reasons for otherwise promising materials to fail technological translation. The enduring state-of-the-art for establishing these properties essentially remains make-and-break testing, which is costly and provides information only at the end of the materials development process. Recent developments in automated reaction prediction potentially provide the means of reversing this paradigm so that stability properties and degradation pathways can be designed like other functional material properties. In this talk I will highlight our group's recent work developing methods for predicting reaction outcomes and how they have been applied to battery electrolytes. The second half of the talk will discuss machine learning approaches to the closely related problem of identifying degradation products on the basis of typical spectral information sources.

Gabriel Burks
University of Notre Dame
Chemical and Biomolecular Engineering

Exploring the Nanoscale: In-situ TEM and Multimodal Characterization of Soft Matter

The pursuit of advanced materials with tailored properties has guided extensive research into polymer crystallization and functional material development. Here we introduce the foundation of our new research program focused on these domains by drawing inspiration from nature's complex structural models and harnessing the power of multimodal characterization techniques, with a particular focus on in-situ transmission electron microscopy (TEM).

Nature has provided a wealth of intricate structural designs, such as the hierarchical arrangements found in many biological systems. By investigating and emulating these complex natural structures, we seek to expand our understanding of classical polymer crystallization processes and develop new synthetic processing methods, and novel functional materials with enhanced properties. In-situ TEM stands as a pivotal tool in this investigation, offering real-time insights into the dynamic evolution of materials at nanoscale dimensions. By monitoring and manipulating polymer crystallization processes within the TEM environment, we gain unprecedented control over nucleation, growth, and morphology. This allows for the direct observation of critical events, including lamellar formation, spherulite growth, and defect generation, offering crucial data for mechanism validation and eventual smart molecular assembly.

Adopting a multimodal characterization approach further enriches our research by coupling TEM with complementary techniques, such as atomic force microscopy, X-ray diffraction, thermal analysis, and various spectroscopy, which enables us to achieve a comprehensive understanding of the structural and chemical aspects of soft material systems. This approach enables our identification of key parameters governing crystallization kinetics and eventual material performance.

Through the integration of natural design principles, in-situ TEM methods, and multimodal characterization techniques, we aim to: 1) elucidate the underlying mechanisms of classical polymer crystallization phenomena, 2) enable new modes for materials processing and development, and 3) better understand the assembly and structural variance of proteins associated with degenerative brain disease.

Ultimately, our interdisciplinary research program not only advances our fundamental understanding of materials science but also paves the way for innovative applications across various industries, including energy, healthcare, and human performance.

Yichen Wu
Ohio State University
Chemistry

Organic-Inorganic Lead Iodide: from Machine Learning to Materials Design

Low-dimensional organic–inorganic lead halides provide an intriguing platform in using organic cations to design materials and properties. My talk introduces a machine learning approach to predict perovskite dimensionality, drawing from ammonium cation features. We also uncover the role of hydrogen bonding-induced secondary structures in shaping hybrid organic lead iodide compounds, offering fresh views into structural control. In the realm of materials design, we present viologen-based lead iodide as a stable and versatile photoelectrode, enabling solar energy conversion in polar solvents. Lastly, we explore water-stable chiral organic-inorganic lead iodide perovskites derived from chiral viologens, promising applications in circular photodetectors.

Shelley Claridge
Purdue University
Chemistry and
Biomedical Engineering

Plenty of room at the top: hierarchical chemical patterning of soft materials

Many problems in modern materials chemistry require highly structured chemical environments at near-molecular scales, integrated into larger micro-to-macroscopic constructs — ranging from nanoelectronics to ligand clustering in biology. However, approaches that are successful at achieving molecular-scale control are often difficult to extend across length scales, or into challenging chemically heterogeneous environments required for real function. Here, we describe a surprisingly robust and scalable route to achieve nm-to-macroscopic chemical patterning of materials based on amphiphilic striped phases, which can be assembled on 2D materials, then polymerized to lock the chemical pattern in place within a 1-nm-thick layer structure. Recently, we have shown that these patterns can be transferred to soft, amorphous materials including PDMS and hydrogels. The transferred surface layer of fully extended, relatively rigid polydiacetylenes with functional headgroups confers both chemical and mechanical function, creating new opportunities for nanostructured material design. We will discuss the relationship between structure, assembly, and reactivity in the molecular template layer, as well as applications in directing assembly of high-aspect-ratio inorganic nanocrystals and in designed cell scaffolds for regenerative medicine.

Meenal Datta
University of Notre Dame
Aerospace and Mechanical
Engineering

Abnormal Mechanics in Brain Tumors: Implications for Hydrogel-Based Models

Patients suffering from glioblastoma – the deadliest primary brain tumor in adults – have a dismal survival of less than 2 years despite aggressive available treatments. Immunotherapy, which has revolutionized the treatment of other solid tumors, fails to benefit the majority of glioblastoma patients. The tumor microenvironment may be largely responsible for this poor response, as it harbors mechanopathologies that drive disease progression and treatment resistance. One such feature is “solid stress” – a mechanical force originating from cells and extracellular matrix – that can compress blood vessels, induce hypoxia and immunosuppression, and hinder immunotherapy delivery and efficacy. Confined and compounded within the rigid skull, solid stress from brain tumors like glioblastoma can also cause debilitating neurological dysfunction. I will present findings from patients and mouse models of glioblastoma that show how solid stress: i) can be measured and/or applied in vivo, ii) can damage the healthy brain tissue surrounding the tumor, and iii) can be targeted to restore neurological function and overcome resistance to immunotherapy. Finally, I will discuss our ongoing efforts to engineer physiologically-relevant glioblastoma models using hydrogels.

You-Yeon Won
Purdue University
Chemical Engineering

Advancing a Novel Polymer Lung Surfactant (PLS) Therapy for ARDS Treatment through Polymer Physics Research

Acute Respiratory Distress Syndrome (ARDS) presents a significant threat, affecting approximately 200,000 patients each year in the United States. ARDS can arise from various underlying causes, including infections such as COVID-19, which compromise the functionality of native lung surfactant. This disruption leads to a critical reduction in blood oxygenation, ultimately culminating in multiple organ failure. Despite the pressing need for effective treatment, therapeutic surfactant formulations have, thus far, yielded disappointing outcomes. Clinical trials involving lipid-based lung surfactants for ARDS treatment, whether originating from animals or synthesized, have not demonstrated efficacy.

Our laboratory has embarked on an innovative path, diverging from traditional lipid/protein-based approaches. We have harnessed the potential of synthetic polymers as the active therapeutic agent to regulate the alveolar epithelium surface tension. This novel direction has resulted in the creation of an amphiphilic block copolymer micelle formulation. Importantly, our formulation exhibits heightened therapeutic efficacy in murine models of acute lung injury, outperforming clinically accessible animal-derived surfactants. A key strength of our polymer-based formulation lies in its ability to intentionally form an insoluble monolayer at the alveolar air-water interface. Remarkably, this monolayer remains resistant to deactivation caused by serum proteins and inflammatory enzymes, even under conditions of lung injury.

In this presentation, I will delve into the trajectory of our polymer physics research efforts spanning several years. These endeavors have paved the way for the groundbreaking development of a pioneering Polymer Lung Surfactant (PLS) therapy for ARDS treatment.

Tengfei Luo
University of Notre Dame
Aerospace and Mechanical Engineering

Discover Thermally Conductive Polymers Using Active Learning

Thermal conductivity (TC), as an important transport property of polymers, can be improved when subject to strain, which can help align polymer chains. However, the discovery of high TC polymers is time-consuming and without guarantee of success. In this work, we employ an active learning scheme to speed up the discovery of high TC polymers. Polymers under strain were simulated using molecular dynamics (MD) and their TCs were calculated. A Gaussian Process model is then trained to screen the PoLyInfo database, and the predicted mean TCs and uncertainties are used towards an acquisition function to recommend polymers for MD labeling. The TC of these selected polymers is then calculated using MD simulations. The obtained data are then added to the training set to start another iteration in the active learning cycle. Through a few cycles, we were able to identify strained polymers with TC much better than the original dataset. This active learning strategy is generalizable to a broad range of materials discovery and design.

Jonathan Whitmer
University of Notre Dame
Chemical and Biomolecular Engineering

Entropy-enhanced Phase Separation in Polyelectrolyte Solutions

Liquid-liquid phase separation is commonplace in biological systems, driven by a combination of specific interactions, charge distributions and crowding. Despite this, the influence of crowding in driving phase separation in confinement is not well understood. I will discuss recent investigations by my group developing a molecular simulation model for polyelectrolyte suspensions in the presence of crowding agents, and discuss the implications for related systems.

Alexander Wei
Purdue University
Chemistry and Materials Engineering

Tunable Rigidochromism of Copper–Pyrazolate Complexes

Copper(I) ions and pyrazoles can self-assemble into macrocyclic clusters with strong solid-state phosphorescence at ambient temperatures. We are investigating a series of tetranuclear Cu–pyrazolate (Cu_4pz_4) complexes whose luminescence relies on a cluster-centered triplet state (^3CC), and whose energies are influenced by substituents far from the Cu_4 core. These remote substituent effects are steric in nature and support a tunable rigidochromism with emissions ranging from yellow to deep blue, confirmed by TD-DFT calculations. As pyrazole ligands increase in structural complexity, polymorphs with different luminescent wavelengths emerge that allow rigidochromic behavior to be tuned by extrinsic physical and chemical stimuli.

#	Poster Title and Authors
1	“Unraveling Origin-Dependent Exosome Uptake and Cargo Release using Chiral Graphene Quantum Dots” by Gaeun Kim, Runyao Zhu, Youwen Zhang, Hyunsu Jeon, and Yichun Wang*
2	“Near Quantitative Preparation of Short, Single-Stranded DNA Circles” by Victoria E. Paluzzi, Cuizheng Zhang, and Chengde Mao
3	“Molecular Modeling of Organic Mixed Ionic-Electronic Conductors” by Xixian Yang, Kejie Zhao
4	“Characterizing Sulfur Copolymer Composite Cathodes for All-Solid Batteries” by Piyush Deshpande, Dr. Jennifer L. Schaefer
5	“Surface fuctionalization of soft polyacrylamide for tissue engineering” by Teah Tirey, Shelley A. Claridge
6	“Underwater Bonding with a Bio-based Adhesive from Tannic Acid and Zein Protein” by Paige E. Kertes, Peter E. Christ, Racheal V. Fisher, Logan J. Miles, Jonathan J. Wilker, and Gudrun Schmidt
7	“Enhancing the Targeting Efficacy of Endothelial Colony Forming Cells for Renal Regeneration via Kidney-targeted Liposomal Nanoparticles” by Brenda Cruz Gonzalez, Eva Hall, Sanjoy Saha, Fei Fan, Donny Hanjaya-Putra
8	“Active Learning Exploration of Thermally Conductive Strained Polymers” by Renzheng Zhang, Jiaxin Xu, Hanfeng Zhang, Tengfei Luo
9	“X-Ray Triggered Drug Release from Paclitaxel-Loaded PEG-PL(G)A-Coated Radioluminescent Nanoparticles – Effects of Glycolide Incorporation, Polymer Molecular Weights, and the Fractionated Radiation Doses” by Sung-Ho Shin, Dhushyanth Viswanath, Kaustabh Sarkar, Samruddhi Patil, Mustafa Ahmed, Jianguo Mei, You-Yeon Won
10	“Bioinspired Dissipative Supramolecular Hydrogel from Dynamic Host–Guest Networks” by Krishnendu Jalani, Bo Su, Christopher Addonizio, Dongping Liu, Matthew J. Webber
11	“Strain-stiffening Zwitterionic Hydrogels” by Sonu Kizhakkepura, Le Zhou, John Klier, Todd Emrick, Shelly Peyton
12	“Shape-dependent Surface Mechanical Behavior of Polystyrene–poly(ethylene glycol) (PS–PEG) Micelles” by Taesuk Jun, Daniel Fesenmeier, You-Yeon Won*
13	“Influence of comonomer sequence architecture on paclitaxel release and degradation behaviors in Poly(Lactic-Co-Glycolic Acid) microparticles” by Samruddhi Patil, Dr. You-Yeon Won
14	“A Non-Equilibrium Steady State Host-Guest Cross-linked Hydrogel” by Connor Schmidt, Matthew Webber
15	“Polymer-dendrimer hybrids: drug delivery and adhesion” by Alexandre Lancelot, Jonathan Wilker, Teresa Sierra
16	“Guiding Material Design to Harness Unsteady State Transport Phenomena for Selective Solute Recovery” by Jonathan Aubuchon Ouimet, Alexander W. Dowling, William A. Phillip.
17	“Stimulated Biomaterials for understanding the biogenesis of Extracellular Vesicles (EVs)” by James Johnston, Yun Young Choi, Gaeun Kim, Hsueh-Chia Chang, Nosang V. Myung, and Yichun Wang
18	“Soft Matter-based Platform for High-Yield and High-Throughput Engineered Organoid Culture.” by Hyunsu Jeon, Yichun Wang
19	“Stereochemically Induced Electronic and Magnetic Properties in Non-Conjugated Radical Polymers” by Hyunki Yeo, Cole Sorenson, Hamas Tahir, Yun-Fang Yang, Frank Leibfarth, Bryan Boudouris
20	“Blocking tau transmission by biomimetic graphene nanoparticles” by Runyao Zhu, Kamlesh M. Makwana, Youwen Zhang, Benjamin H. Rajewski, Juan R. Del Valle, Yichun Wang
21	“Practical Approaches to Bottom-Up Coarse-Graining for Liquid Crystalline Conducting Materials” by Dylan Fortney, Brett Savoie
22	“Investigating the Nucleation and Growth Mechanism of Coiled-Coil Peptide Crystals” by Andrew Encinas, Jean Chmielewski
23	“Leveraging Dynamic-Covalent Bonds for Glucose-Responsive Peptide Structures” by Emily DeWolf, Elizabeth Power, and Matthew Webber, PhD
24	“2D Hemidirected Lead Organic Chalcogenide” by Hanjun Yang, Sagarmoy Mandal, Yoon Ho Lee, Jee Yung Park, Han Zhao, Chongli Yuan, Libai Huang, Ming Chen, Letian Dou
25	“Artificial Eye Based on Photon-Modulated Electrochemical Doping” by Ke Chen, Hang Hu, Inho Song, Habtom B. Gobeze, Won-June Lee, Ashkan Abtahi, Kirk Schanze, and Jianguo Mei
26	“Phase-Resolved Electrogenerated Chemiluminescence with a Single Luminophore” by Brady R. Layman, Jeffrey E. Dick
27	“Electrochemically-Initiated Macromolecular Assembly: Dispersion Electropolymerization in Aqueous Microdroplets” by Myles Q. Edwards, Joshua Reyes-Morales, Saptarshi Paul, Jeffrey E. Dick
28	“Probing the kinetics of cerium (IV) extraction by tributyl phosphate using microfluidics” by Megan L. Hill and Dr. Anna G. Servis
29	“Anodic Electrodeposition of Iridium Oxide from Aqueous Nanodroplets” by Saptarshi Paul, Joshua Reyes-Morales, Kingshuk Roy and Jeffrey E. Dick

#	Poster Title and Authors
30	“Wafer-scale Photosensor Arrays via Synthesis of 2D Perovskite Nanosheet Crystals Using Spray Coating” by Yoon Ho Lee, Won-June Lee, Jee Yung Park, Gangsan Lee, Hanjun Yang, Jianguo Mei, Letian Dou
31	“Optimization of Photosensitive characteristics of OECT” by Adit Batra, Ke Chen
32	“Development of a supramolecular hydrogel for prime-boost vaccine delivery” by Audrey Hansrisuk, Matthew J. Webber
33	“Polybenzimidazole-based Membranes with Semi-Interpenetrating Network (s-IPN) Structures for High-Temperature H2/CO2 Separation” by Mengdi Liu, Si Li, Ruilan Guo
34	“Ln(III) mediated assemblies with coiled coil trimeric peptide” by Anna V. Pavlishchuk, Andrew Encinas, Michael Jorgensen, Jean Chmielewski
35	“Depolymerizable Polyolefins with Intrinsically-Weakened Carbon-Carbon Bonds” by Qixuan Hu
36	“Anodic Coloring Electrochromism (ACE) Polymer Color Prediction via Machine Learning” by Jianing Zhou
37	“Towards large-area perovskite solar cells via doctor blade coating” by Wenzhan Xu, Yoon Ho Lee, Yuanhao Tang, Jiaonan Sun, Prashant Kumar, Prof. Jianguo Mei and Prof. Letian Dou
38	“Solid Organic Charge-Transfer Composites as Lithium-Ion Battery Electrolytes” by Lingyu Yang, Jennifer Schaefer
39	“Dissipative Non-Equilibrium Host–Guest Hydrogels Regulated by Consumable Fuels” by Bo Su, Teng Chi, Zhou Ye, Yuanhui Xiang, Ping Dong, Dongping Liu, Christopher J. Addonizio, Matthew J. Webber
40	“Experimental and computational analysis of the injection-induced mechanical changes in the skin microenvironment during subcutaneous injection of biologics” by Yingnan Shen, Sameep Rajubhai Shah, Kejie Zhao, Bumsoo Han
41	“Reaction Mechanism and Network for Oxidative Degradation of Polyethylene Glycol” by Lawal A. Ogunfowora; Lyudmila V. Slipchenko; Brett M. Savoie
42	“Sustained Release of Glucagon Like Peptide-1 (GLP-1) From Injectable Hydrogels Protect Rats From Hyperglycemia” by Weike Chen, Sijie Xian, Bernice Webber, Dongping Liu, Matthew Webber
43	“Nanoscale structure control and high-fidelity characterization of molecular layer-by-layer assembled thin film” by Jizhou Jiang, Garam Lee, Casey O’Brien, Bryan Paulsen, Jennifer Schaefer
44	“Transparent Electrochromic Polymers and Devices with Ultrahigh Optical Contrast Ratio” by Zhiyang Wang
45	“Single-cell mechanical analysis reveals viscoelastic similarities between normal and neoplastic brain cells” by Onwudiwe, Killian; Najera, Julian; Holen, Luke; Burchett, Alice A.; Rodriguez, Dorielis; Zarodniuk, Maksym; Siri, Saeed; Datta, Meenal
46	“Development of Composite Block Copolymer Adsorptive Membranes on a Nonwoven Support” by Annabelle Li, William Phillip
47	“Functional Analysis of Vascular Networks in Stem Cell Organoids” by Dominique Gramm, Donghyun Jeong, Donny Hanjaya-Putra, Christopher Patzke