Materials Research Laboratory University of California Santa Barbara Materials Research Outreach Program 2025

Corwin Pavilion, Wednesday January 29th and Thursday January 30th 2025

Program and Speaker Bios, and Poster Abstracts

UC Santa Barbara Materials NRRL Research Laboratory

NSF Materials Research Science and Engineering Center [DMR-2308708]

Program: Wednesday January 29th

8:45 am	Opening Remarks by College of Engineering Dean Umesh Mishra		
Session Chair: Raphaële Clément			
9:00 am	Nadia Léonard	Electrochemical Carbon Dioxide Incorporation into Multi-	
	(UCSB)	Carbon Products	
9:30 am	Tyler Mefford	Understanding the Local Chemistry of Water Oxidation	
	(UCSB)	Catalysts	
10:00 am		Break	
Session Chair: Ram Seshadri			
10:30 am	Cassidy Tobin	Reversible and Size-Controlled Assembly of Reflectin Proteins	
	(UCSB)	Using Molecular Photoswitches	
11:00 am	Sam Wilken	DNA Liquid Droplets Embedded in Cytoskeletal Networks	
	(UCSB)		
11:30 am	Zoe Liberman	Infants' Social Expectations and Social Learning	
	(UCSB)		
12:00 noon	Lunch		
Session Chair: Angela Pitenis			
1:30 pm	Haley Beech	Immiscible Polymer Blend Compatibilization through Pendant	
	(UCSB)	Ionic Interactions	
2:00 pm	Parker Morris	Scalable Synthesis of Degradable Copolymers Containing α -	
	(UCSB)	Lipoic Acid via Miniemulsion Polymerization	
2:30 pm	Break		
Session Chair: Chris Bates			
3:00 pm	Tim Long (ASU)	Cheetham Lecture: Designing Advanced Macromolecules for	
		Advanced Manufacturing: Balancing Reactivity, Rheology,	
		Resolution, and Rate (4 Rs)	
4:15 pm	Reception and posters		

UC Santa Barbara Materials NREsearch Laboratory

NSF Materials Research Science and Engineering Center [DMR-2308708]

Program: Thursday January 30th

Session Chair: Meredith Murr			
9:00 am	Rachel Segalman	Welcome, and Overview of the Sustainable Products and	
	(UCSB)	Packaging Consortium	
9:30 am	Chris Bates	UCSB's Strengths in Polymers/Upcycling	
	(UCSB)		
9:50 am	Scott Shell	UCSB's Strengths in Formulations	
	(UCSB)		
10:10 am	Break		
Session Chair: Rachel Segalman			
10:30 am	Roland Geyer	UCSB's Strengths in Life-Cycle Analysis/Techno-Economic	
	(UCSB)	Analysis	
11:00 am	Steven Arturo	Don't Let it go to Waste - Plastics and the Circular Economy	
	(Dow)		
11:30 am	Karla Mora	Investing in Innovation: Building Sustainable Value Chains for	
	(Alante Capital)	Consumer Brands	
12:00 noon	Lunch		
Session Chair: Meredith Murr			
1:30 pm	Matt Wagner	Material Sustainability from Feedstock to Finished Product	
	(P&G)		
2:00 pm	Lawrence Fischel	Sustainable Packaging Design Successes and Challenges	
	(Clorox)		
2:30 pm	Tal Margalith	Overview of BioPACIFIC MIP	
	(UCSB)		
3:00 pm	Faculty Panel		
3:45 pm	Break		
4:00 pm to	Closed Session for Select Invitees: Panel-Facilitated Discussion about Consortium		
5:00 pm	Structure		

UC Santa Barbara Materials NRRL Research Laboratory

NSF Materials Research Science and Engineering Center [DMR-2308708]

Tim Long received his Ph.D. in Chemistry from Virginia Tech, and he subsequently joined both Eastman Kodak and Eastman Chemical companies for eight years upon graduation. He joined the faculty in the Department of Chemistry at Virginia Tech, where he also served as the Director of the Macromolecules Innovation Institute until 2019.

In 2020, Prof. Long accepted an interdisciplinary faculty position across the School of Molecular Sciences (SMS) and the School for Engineering Matter, Transport, and Energy (SEMTE) at Arizona State University (ASU) where he launched and now leads the Biodesign Center for Sustainable Macromolecular Materials and Manufacturing (BCSM3).

In addition to over 440 peer-reviewed publications, his research awards include the 2023 3M Excellence in Adhesion Award, 2022 Paul J Flory Award, 2020 Virginia Outstanding Faculty Award, 2015 Virginia Scientist of the Year, 2010 Virginia Tech Alumni Research Award, ACS PMSE Collaborative Research Award, PSTC Carl Dahlquist Award, 2019 ACS Rubber Division Thermoplastic Elastomer Award, and the ACS POLY Mark Scholar Award.

His most recent research efforts address the need for tailored advanced macromolecules for advanced manufacturing (3D printing), including vat photopolymerization, direct ink write, binder jetting, powder bed fusion, and melt extrusion. His research ranges from controlled polymerization processes for block copolymers to high performance engineering polymers for emerging technology with a lens of earth sustainability.

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Nadia Léonard received her Ph.D. in chemistry from Princeton University where she was an NSF Graduate Research Fellow. Her doctoral research focused on developing earth-abundant transition metal catalysts for site-selective functionalization of hydrocarbon feedstocks. She then pursued postdoctoral research at the University of California, Irvine where she investigated electric field effects at transition metal complexes as a UC President's Postdoctoral Fellow with Professor Jenny Yang.

She joined the faculty at UC Santa Barbara as an Assistant Professor in the Department of Chemistry & Biochemistry in 2023. Her research is centered on the design of inorganic molecular complexes and materials with unique physical and catalytic properties for applications toward energy storage and conversion, pollutant sensing, and sustainable catalysis.



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Tyler Mefford received his B.S. in Chemistry in 2012 from Stanford University and Ph.D. in Chemistry in 2016 from the University of Texas at Austin. After a postdoc and Senior Staff Scientist position in Materials Science & Engineering at Stanford, he joined the Department of Chemical Engineering at UC Santa Barbara as an Assistant Professor in January 2024.

His lab works at the intersection of engineering, chemistry, and materials to develop redox-active polymers and inorganic electrode materials for applications in electrochemical energy conversion, storage, and chemical separations. Understanding of the non-equilibrium properties of electrochemical systems and reaction mechanisms across time and length scales is aided by a focus on device development, operando spectroscopy, microscopy, and scattering techniques, and computational methods.

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Cassidy Tobin is a fifth-year Ph.D. candidate in the Chemical Engineering department at UC Santa Barbara. She received her B.S. in Chemical Engineering from Georgia Institute of Technology, where she worked under Professor Paul Kohl on the synthesis and applications of low-ceiling temperature polyaldehydes. During her undergraduate studies, Cassidy also worked as a co-op student for Avient Corporation, where she applied lean manufacturing strategies and developed material testing methods for composite materials.

Currently, Cassidy is advised by Professor Javier Read de Alaniz and is developing novel, light-responsive molecules that reversibly assemble disordered proteins, such as the reflectin protein. By achieving reversible photocontrol of protein assembly, her research aims to enable the creation of life-like systems with tunable material properties.



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Sam Wilken is an experimental physicist interested in combining precision microscopy, large-scale simulation, and nanoscale biomolecular design to investigate the far-from-equilibrium organizational mechanisms by which biology has evolved unique disordered materials. Currently, he is a postdoc at the University of California, Santa Barbara, working on experimental model systems of biomolecular phase separation with Omar Saleh.

Sam earned his Ph.D. in physics from New York University, working on absorbing-state phase transitions in sheared suspensions, random sphere packings, and hyperuniformity with Paul Chaikin. He began his adventure in soft matter physics by working on dense suspension impact and "evolved" materials with Heinrich Jaeger while earning his BA in physics (with honors) at the University of Chicago.

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Zoe Liberman is an Associate Professor in the Department of Psychological and Brain Sciences at UCSB. Her research focuses on the development of social cognition: how babies and young children learn about--and learn from--people. She is most interested in the origins of human understanding of social relationships, including friendship, group membership, and family.

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Haley Beech is currently a postdoctoral researcher in the groups of Professors Rachel Segalman and Craig Hawker at UC Santa Barbara. Her current research is focused on synthetic functionalization and processing for commodity polymer compatibilization and improved recyclability. Haley earned a Ph.D. in chemical engineering from MIT under the guidance of Professor Bradly Olsen, where her research was focused on relating single polymer chain behavior and topology to macroscopic properties in polymer networks. She received her B.S. in chemical engineering from the University of Minnesota, where she researched the phase behavior of di-block copolymer blends with Professor Frank Bates. When not thinking about polymers, Haley is probably running on the beach or reading in the sun.

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Parker Morris graduated from the Robert D. Clark honors college at the University of Oregon in 2021 with a bachelor's degree in chemistry. He is currently a 4th year graduate student studying degradable polymers with Professors Chris Bates and Javier Read de Alaniz. In his eyes, finding a solution to the global plastic crisis is the paramount challenge of polymer chemists and he has spent the last four years studying this problem.

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Rachel A. Segalman is the Edward Noble Kramer Professor and a Distinguished Professor at University of California, Santa Barbara. Her laboratory works on semiconducting block polymers, polymeric ionic liquids, and hybrid thermoelectric materials. She is the associated director of the Center for Materials for Water Energy System; a DOE EFRC, an associate editor of ACS Macro Letters, and co-editor of the Annual Review of Chemical and Biomolecular Engineering.

Segalman studied chemical engineering at University of Texas at Austin (UT). She received her Ph.D. in 2002 from UCSB where he worked under the supervision of Edward J. Kramer. After completing her Ph.D., Segalman was a Chateaubriand postdoctoral fellow in Strasbourg working under Georges Hadziioannou.

In 2004 Segalman joined Chemical Engineering at University of California, Berkeley, and the Lawrence Berkeley National Laboratory (LBL) Materials Science Division. In 2013 she was appointed as the acting director of LBL Materials Science Division. Segalman was recruited to UCSB in 2014 as the Kramer Professor of Materials in the Departments of Chemical Engineering and the Materials Department.



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Chris Bates received his B.S. in Chemistry from the University of Wisconsin, Madison and his Ph.D. in Chemistry, University of Texas at Austin working under the guidance of C. Grant Wilson. After carrying out postdoctoral research in the group of Robert Grubbs at Caltech, he joined the Materials Department at UC Santa Barbara in 2016. He currently holds appointment as Associate Professor in the Departments of Materials, Chemistry & Biochemistry and Chemical Engineering.

Research in the Bates group sits at the intersection of chemistry and materials science, leveraging synthetic and physical experimental techniques to design, create, and probe the properties of soft matter. Current endeavors span a variety of topics including block polymer self-assembly, new elastomeric materials, and thin film patterning.

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Scott Shell is the Myers Founder's Chair in Chemical Engineering Professor and Vice Chair for Graduate Education in the Department of Chemical Engineering University of California Santa Barbara. He received his BS degree in Chemical Engineering from Carnegie Mellon University and 2000, and his PhD from Princeton Chemical Engineering, Princeton University, advised by P. G. Debenedetti and A. Z. Panagiotopoulos. He was a Postdoctoral Scholar in the Department of Pharmaceutical Chemistry, University of California San Francisco under K. Dill before starting his faculty career at UCSB in 2007.

The Shell lab uses theoretical and atomistic simulation methods, in concert with statistical learning, to understand how fundamental molecular interactions modulate the thermodynamic and kinetic behavior of nanoscale systems, and how these interactions might be manipulated through design of new processes and molecular architectures.



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Roland Geyer is a Professor at the Bren School of Environmental Science and Management, University of California at Santa Barbara. Prior to joining the Bren School he held research positions at the Centre for Environmental Strategy (University of Surrey, UK), the Centre for the Management of Environmental Resources (INSEAD, France), and was a consultant in financial risk management for AMS (now part of CGI) in Germany. Since 2000 he has worked with a wide range of governmental organizations, trade associations, and companies on environmental sustainability issues. In his research he uses the approaches and methods of industrial ecology, such as life cycle assessment and material flow analysis, to assess pollution prevention strategies based on reuse, recycling, and material and technology substitution. Roland also combines these approaches with research methods from other disciplines to study the relationship between environmental performance, economic viability, and technical and operational feasibility of pollution prevention strategies. His overarching goal is to help develop the knowledge, tools, and methods necessary to reduce the environmental impact from industrial production and consumption. Roland has a graduate degree in physics from the Technical University Berlin and a PhD in engineering from the University of Surrey.

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Lawrence Fischel PhD is Senior Scientist, Modeling & Simulation – The Clorox Company, where he has been developing and implementing multifaceted, multiscale M&S approaches in support of several Clorox business units, such as Cleaning and Foods. He has been with Clorox for eight years. In this time, he has taken innovative experimental or computational roles in process, product, and packaging development. In his current role, Lawrence is responsible for developing Finite Element Analysis (FEA) approaches for packaging evaluation in support of the technical sustainability pipeline for packaging that will help Clorox meet its 2030 sustainability goals while delivering innovation and/or cost savings for the company. Lawrence earned a Ph.D. in Chemical Engineering from UC Berkeley after a B.S. in Chemical Engineering from UCLA. He uses his expertise to explore and vet materials, designs, and technologies that help bring consumer relevant products to life while bringing positive change to the planet.

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Steve Arturo PhD, is a Principal Research Scientist in the Formulation, Automation, and Materials Sciences group within Core R&D at The Dow Chemical Company. Steve is the technical leader of Computational Materials Sciences, applying physics-based and hybrid models to build a bridge between molecular-level phenomena and macroscopic properties of formulations and materials. Steve works across modeling groups in chemistry, engineering, and data science to provide holistic digital solutions to colleagues and customers of Dow. Steve's academic training is in applied mathematics and chemical engineering, specifically solution thermodynamics for the computation of properties of pure species and mixtures. While at Dow, Steve learned polymer reaction engineering while working on internal projects and in an external collaboration with Northwestern University. Steve continues his work in miscibility modeling and in advanced structure-property relationships using kinetic Monte Carlo methods for detailed polymer architecture. Steve's work has resulted in the development of several new products and has debottlenecked manufacturing processes.

More recently, Steve has applied domain knowledge within active learning methods to decrease the amount of experimentation and to reach experimental objectives more quickly than using traditional methods. Steve's organizational work inside of Dow includes leading technical leaders in data science, contributing to strategy development for digitalization efforts across Dow R&D, and partnering with professional organizations (AIChE, ACS, CoMSEF), external companies (IBM), journals (ACS Engineering Au), and universities (UCSB, UIUC). Steve takes care in mentoring graduate students and colleagues to have a greater impact in sustainability and digitalization efforts. Outside of Dow, Steve volunteers at the Attic Youth Center, Philadelphia's only independent LGBTQ youth center. Steve earned his B.S. and Ph.D. at the New Jersey Institute of Technology. In his 17 years at Dow, he has four granted patents, authored 16 publications in peer-reviewed journals, and has given dozens of external presentations related to his research program. Steve has recently won the BIG Innovation and ICIS awards for collaborative work in providing digital solutions to Dow customers.

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Matt Wagner is a Director in Research & Development at The Procter & Gamble Company in Cincinnati, Ohio. Matt's career has spanned analytical chemistry and technology and product development across cleaning and hygiene categories and brands. Matt's current focus is on the development of high performing and sustainable materials for P&G's products and brands.

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Karla Mora is the Founder and Managing Partner of Alante Capital, a VC fund focused on enabling a circular and decarbonized future for the apparel, footwear, and home goods industries. Launched in 2016, Alante creates a collaborative space for startups, corporates, and investors to support solutions to pressing global problems. The fund invests in early-stage innovations that address systemic issues across consumer industries.

A development economist by training, Karla has dedicated her career to reforming production practices to improve working conditions and protect the environment. Before launching Alante, her experience included investing in early-stage social enterprises in emerging markets, working on supply chain reform in Afghanistan, and with the UN Sustainable Commodity Initiative for the coffee sector. She currently serves on the boards of Mango Materials, FIT:MATCH.ai, and Sway and is a Bren Eco Entrepreneurship Advisory Council member.

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Tal Margalith received his PhD in Materials from UCSB in 2002, in the field of Gallium Nitride optoelectronics. After graduating, he spent 10 years in the industry: first in the R&D division of Philips Lumileds Lighting, then at UCSB-spinoff Soraa as the Director of the Process Engineering arm of the company's Operations Division.

Tal serves as the Executive Director for Scientific Initiatives and Innovation at the California NanoSystems Institute (CNSI), where he works to strengthen corporate relations and technology outreach, facilitate technology translation from academia to industry, and promote new multi-PI and multi-campus initiatives for science and engineering at UCSB. Tal oversees the shared-use facilities, runs the startup-focused CNSI Technology Incubator program, and serves as the Industry Liaison for the NSF Quantum Foundry and the Executive Director for BioPACIFIC MIP.

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Polymer Sequence Alters Sensitivity and Resolution in Chemically-Amplified Polypeptoid Photoresists

C. P. Adams^a, C. Henein^a, C. Yuan^b, C. K. Ober^b, and R. A. Segalman^a ^aUniversity of California, Santa Barbara ^bCornell University

Polymer photoresists have long played a critical role in the fabrication of microelectronic devices. However, significant challenges with stochastics and sensitivity have arisen as state-of-the-art "extreme ultraviolet" (EUV, 13.5 nanometer wavelength) lithography tools now allow for patterning of sub-10 nm features. To address these issues, we have developed polypeptoid-based photoresists to probe the effects of polymer sequence and chain length on patternability. Traditional polymers have inherent dispersities in molecular weight, composition, and sequence. These are compounded by material inhomogeneities in photoresist formulations and poor EUV photon absorption, contributing to unacceptable patterning defects. Sequence specificity of the peptoid system eliminates these variations, and a tunable synthesis involving primary amines allows for the incorporation of a vast range of functionalities. In this study, we investigated the impacts of both chain length and sequence on pattern contrast and resolution. Contrary to traditional models that predict equivalent patterns for materials of identical composition, we found that polymer sequence can substantially impact patterning resolution and sensitivity. These findings open up a new design space for polymeric photoresists as we move towards future studies of how the placement of individual functionalities can improve patterning performance.

Synthetic Study and Characterization of Zwitterionic-Gyroid Structure

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The gyroid structure, a microphase-separated morphology with a three-dimensional bicontinuous architecture, shows promise for various applications, including matter transport and optical devices, particularly when combined with zwitterionic moieties. Here, we explore three approaches to achieve zwitterionic-gyroid structures:

• High-Throughput Study of Zwitterionic BCP Morphology Behavior:

Using well-fractionated BCPs containing active ester groups, we conducted systematic studies of zwitterionic BCP morphologies.¹⁾ The BCPs were functionalized with amine-containing sulfobetaine, and the resulting morphologies were characterized by SAXS.

• ABC-Triblock Copolymer Templates for Structured Zwitterionic Films:

Building upon Li et al.'s demonstration of cross-linked BCPs, we utilized their epoxide-containing BCP system for post-functionalization.² By introducing sulfobetaine with a secondary amine, we successfully functionalized this film while preserving its morphology. The functionalized film exhibited enhanced water uptake compared to the original structure.

• Gemini-Structured Zwitterionic Liquid Crystals:

Gemini- structured zwitterionic liquid crystals (LCZIs) are known to form gyroid structures when blended with salts or acids, typically yielding smaller d-spacing than BCPs.^{3,4} We synthesized the imidazolium-type gemini-structured LCZI to enhance functionality.

Acknowledgment: We would like to thank Prof. Ichikawa for providing valuable advice on the synthesis of Gemini- structures.

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Converting a Metal-Coordinating Polymer to a Polymerized Ionic Liquid Improves Li⁺ Transport

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Solid polymer electrolytes made from mechanically robust and nonflammable materials will enable the next generation of Li⁺ batteries with higher power and energy density. However, fundamental limitations in the transport mechanism of conventional polymer electrolytes bar them from attaining marketrelevant Li⁺ conductivity. Herein, demonstrate that conductivity in a highperforming metal-ligand coordinating polymer (PMS-Im) can be substantially improved by chemically modifying its imidazole ligand to imidazolium (PMS-Im⁺). As an ionic liquid functionality, the polymer-bound imidazolium



Imidazolium functionality on polymer electrolyte substantially improves Li⁺ conductivity compared to imidazole functionality.

provides several key advantages: (i) plasticization of the polymer electrolyte to a lower glass transition temperature (T_g), (ii) insensitivity of T_g to the addition of Li salt, (iii) solvation of high salt loadings without trapping Li⁺, and (iv) formation of ion-rich pathways with electrochemically beneficial ion-ion correlations (i.e. a high inverse Haven ratio). As a result, Li⁺ conductivity in PMS-Im⁺ (2.1*10⁻⁵ S/cm) is over an order of magnitude greater than in PMS-Im at 90 °C, and the difference is several orders of magnitude at 30 °C.

Value of PEP as a Model Substrate for Polyolefin Depolymerization and Associated Upcycling Strategies

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The growing emphasis on circular carbon and reducing greenhouse gas emissions in the chemical industry has driven efforts to recover chemical components from plastics for reuse. Partial depolymerization of polyolefins, however, remains challenging due to the complexity of both the materials and the resulting product distributions. While simplifying the problem by using model substrates is a common strategy, some simplifications can overlook critical properties necessary for predictive models. Here, we propose polyethylene-alt-propylene (PEP) as an ideal model substrate for polyolefin depolymerization. PEP retains key characteristics of commercial polyolefins while offering advantages in characterization. Using a fluorinated alumina catalyst, we demonstrate the catalytic depolymerization of PEP and compare its behavior to a commercial polyethylene, highlighting of depolymerization the utility PEP in advancing research.

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New Precursors and Methods for Hard Carbon Anodes in Na-Ion Batteries

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While lithium-ion batteries are ubiquitous in consumer electronics and electric vehicles, their high

cost makes them unattractive for grid-scale energy storage, the demand for which will increase with the adoption of intermittent renewable energy. Na-ion batteries are a promising alternative due to the low cost and earth abundance of sodium, but are limited in capacity and cycle life by poor anode materials. We have investigated novel precursor materials (biomatter, waste plastics, and purpose-built custom polymers) and synthesis methods (conventional furnace heating versus microwave heating) to produce hard carbon anodes with customized, tunable properties. We use Raman, XRD, PDF, and BET to probe the structural motifs of the hard carbons such as disorder, layer spacing, and pore size. Understanding the fine structural details of the hard carbon materials will yield an understanding of Na intercalation mechanisms during battery cycling. We ultimately make Na-



Raman spectra of PVDC derived hard carbon. Integrated intensity I(D)/I(G), here 2.34, quantifies disorder of the material.

ion batteries from our materials, the cycling of which allows us to tie together structure and performance.

- D. Chen, W. Zhang, K. Luo, Y. Song, Y. Zhong, Y. Liu, G. Wang, B. Zhong, Z. Wu, and X. Guo, Hard carbon for sodium storage: mechanism and optimization strategies toward commercialization, *Energy & Environmental Science* 4 (2021), 2244-2262.. DOI: 10.1039/DoEE03916K
- 2. J. M. Stratford, A. K. Kleppe, D. S. Keeble, P. A. Chater, S. S. Meysami, C. J. Wright, P. L. D. S. P. P. G. A. V. M. L. A. S. K., J. W. L. B. M. O. E. T., and C. P. Grey, Correlating local structure and sodium storage in hard carbon anodes: insights from pair distribution function analysis and solid-state NMR, *J. Am. Chem. Soc.* 143 (2021) 14274–14286. DOI: 10.1021/jacs.1co6750.

Making Hydrogels in "Dark Mode": Tuning Hydrogel Structure and Properties Using Time-Modulated Photocuring

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Uncontrolled, photoinitiated radical polymerization is used commercially to create hydrogels across a wide range of applications including coatings, 3D printing, fine particles, and biomedicine. Despite this ubiquity, radical polymerization typically creates complex hydrogel structures that are difficult to control through molecular chemistry alone, leading to empirical optimization of pre-

cursor formulations to engineer their properties. In this work, we demonstrate an alternative approach that uses time-modulated photoinitiation as a processing tool to control the kinetic development of hydrogel structure. Using poly(ethylene glycol) methyl ether acrylate (PEGMEA) as a model linear bottlebrush, and poly(ethylene glycol) diacrylate (PEGDA) as a model hydrogel system, we demonstrate how controlling the time scales of alternating "light" and "dark" photoexposure intervals provides a route to control the molecular weight distribution of active radical oligomers, thereby controlling the topology and structure of crosslinking centers within the emerging network. Gel Permeation Chromatography coupled to Multi-Angle Light Scattering (GPC-MALS) measurements elucidate the impact of this process on the absolute molecular weight of PEGMEA bottlebrushes, whereas small



Periodic photoinitiation allows control over the network topology and the resulting bulk properties of hydrogels synthesized via radical polymerization

angle X-ray/neutron scattering and swelling experiments are used to track the resulting changes in the final PEGDA network structure.¹ The results are rationalized using a detailed kinetic model that predicts the time-evolving molecular weight distribution of crosslinking species within the network.² Ultimately, we show that high-frequency cycling of photoexposure produces a population of long, bottlebrush-like crosslinking centers that act as rod-like reinforcements of the hydrogel network, leading to significantly enhanced strain-stiffening, toughness and extensibility.³ The results demonstrate how time-modulated photocuring can be used as a simple, general, and chemically orthogonal route to control network structure and properties of photopolymerized hydrogels.

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Behavior and Properties of Many Distinct DNA Liquids

A. S. Chaderjian^a, S. Wilken^{a,b}, and O. A. Saleh^{a,b}

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The cell consists of many liquid compartments phase-separated from the cytosol, but also

apparently immiscible with each other. To explore such multi-condensate systems, we have created an artificial mixture of many immiscible biomolecular liquids. Each liquid consists of similar DNA particles, but the distinct liquids remain immiscible due to DNA sequence-specificity. We compare the phase behavior and materials properties of these different liquids, offering insight into the degree of predictability of multi-condensate properties. Additionally, we demonstrate the capability of such a mixture to form a stabilized 2D tissue-like packing of droplets.

This work was partially supported by the MRSEC Program of the National Science Foundation under Award No. DMR 2308708, and by the W.M. Keck Foundation.



Nine distinct, immiscible liquid phases of DNA, distinguishable by fluorescent dyes as well as different tagged fractions. This image was taken nearly 3 days after droplet formation, underscoring the stability of this dense packing.

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Journal of Physical Chemistry, B, 124(40):8888-8895, 2020. DOI: 10.1021/acs.jpcb.0c06911

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Measuring and Modeling Deformations of Topology-Defined Polymers Using In Situ Scattering in a Capillary Rheometer

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Applications of high molecular weight dilute polymers typically involve extreme shear rates that cause nonlinear deformations and chain scission. Although various microscopy methods have successfully resolved single-molecule deformations for specific biopolymer systems, techniques inaccessible these are to conventional, synthetic polymers undergoing deformation in high shear flows. We present new small-angle neutron in situ scattering measurements using a high-shear capillary rheometer¹ to simultaneously characterize the microstructure and rheology of topologically complex polymers. The resulting scattering is interpreted using a new modeling framework, Gram-Charlier analysis of polymer scattering (G-CAPS), that fingerprints nonlinear deformations of polymers through non-Gaussian moments of the segment density distribution.² The method is



Uncovering topology-dependent deformation mechanics of dilute polymer solutions in shear flow using in situ scattering in a capillary rheometer that can reach extreme shear rates $\sim 10^6 \text{ s}^{-1}$.

validated using synthetic data from Brownian dynamics simulations, and applied to capillary rheo-SANS measurements on a series of topology-controlled polymers in high shear rate flows to test the influence of chain topology and extensibility on non-Gaussian polymer deformations. We anticipate that capillary rheo-SANS in combination with G-CAPS will provide powerful new tools to understand and engineer the molecular rheology of polymer fluids.

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Nanofilament Biopolymer Material for Neurodegenerative Disease Screening

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Recreating tau folds that mimic the conformations seen in neurodegenerative diseases also known as tauopathies is crucial for developing diagnostic and therapeutic tools. Screening for disease-specific antibodies, small molecule inhibitors, and positron emission tomography agents necessitates a well-defined and representative amyloid fibril target. To design these agents that target the growing ends of pathological filaments and bind to specific tauopathies, a bottom-up approach of generating synthetic fibers using a small section of tau that spans the R₂/R₃ junction was tested.¹ Rationally designing the peptide with mutations, post-translational modifications (PTMs) and environmental conditions has allowed us to bias the fiber's internal orientation to resemble filament cores as seen from post-mortem samples.

With a library of synthetic fibers accumulating around specific disease targets, the Han lab has developed a "Tau Seeding Kit" (TauSeeK) that can accelerate the agent screening process to find specific binders. These tau replica seeds exhibit similar characteristics to patientderived samples, such as paired helical fiber (PHF) morphology and prion-like properties, and act as templates that guide and stabilize critical parts of tau



Figure 1. A. Monomeric full-length tau found in the brain. B. Folded pathological tau found within neurons. C. *Top*: Corticobasal Degeneration (PDB: 6VH7), close up on residues 295-313 with H299 in cyan, S305 in green and Y310 in pink. *Bottom*: Progressive Supranuclear Palsy (PDB: 7P65), close up on the same residues. D. The morphology of the fibers are shown with negative stain TEM adjacent to the DEER data showing the different conformational populations by measuring the distance between residue 300 and 314 of *top*, pS305 and *bottom*, pY310 synthetic fibers.

to fold and adopt the disease-specific core. Our seeds aggregate tau protein in vitro and in mammalian cells with high efficiency and specificity.² These kits are free from biological debris, highly sequence-specific, and customizable with mutations and PTMs at desired residues, all while being fast to produce. These fibers have been tested for PET radioligand binding and are currently being screened for new antibody affinity.

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Electrostatically Mediated Compatibilization of Immiscible Polymer Blends via a Quaternization Approach

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Electrostatic interactions enable the creation of compatibilized polymer blends with enhanced properties applicable to the recycling of mixed plastic waste. Typically, ionic bonds are formed by either the 1) reversible, counterion free proton transfer process between acid and base groups, or 2) coacervation process upon solution mixing of oppositely charged polymers. Here, we demonstrate the quaternization of tertiary amines (*e.g.*, quinuclidine) with alkyl sulfonates (*e.g.*, ethyl sulfonate)

in creating strong ionic bonds that forces incompatible polymer chains to mix and suppress macrophase separation, generating counterion free compatibilized blends. We showcase this compatibilization strategy with a highly incompatible model system comprising poly(dimethylsiloxane) (PDMS) and poly(methyl acrylate) (PMA) at sparse levels of functionalization (e.g., chain-end and 1 mol% pendant groups). Quinuclidine moieties are installed through the postpolymerization functionalization of PDMS bearing vinyl groups *via* thiol-ene click chemistry. ¹³C-labeled ethyl sulfonate groups are incorporated in PMA through RAFT polymerization, with the quaternization conversion easily tracked by quantitative ¹³C NMR spectroscopy. An increase in optical clarity of the initially turbid, macrophase separated mixture indicates that blend compatibilization is achieved in the presence of sparse ionic bonds created upon quaternization, whereby the phase separated domains are reduced to the nanoscale as elucidated by small-angle X-ray scattering.



The quaternization of tertiary amines with alkyl sulfonates yield strong ionic bonds that compatibilizes immiscible polymer blends at sparse amounts.

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Acidic Conditions Promote Clustering of Cancer Cell Derived Extracellular Vesicles and Enhance their Fusion with Synthetic Liposomes

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Extracellular vesicles (EVs) are endogenous cell-secreted vesicles. Exosomes are a subset of EVs with diameters of 30 to 150 nm which play a key role in intercellular communication. Exosomes are promising cancer chemotherapeutic drug delivery vehicles given that they show low immunogenicity and cell-specific cytosolic delivery of their contents. However, their therapeutic application is limited by inefficient drug loading. Methods for fusion of EVs with drug-loaded synthetic liposomes have been developed to address this. While these methods are more efficient than passive incubation, they risk damage to critical EV membrane proteins or contamination of the EV-liposome hybrid samples with depletant molecules which can hinder delivery or cause side effects. Here we present a weakly perturbative method which uses acidic conditions (pH 5) to enhance fusion of EVs and synthetic, neutral liposomes (NLs) compared to passive incubation at pH 7.4 and 37°C. An adapted Forster resonance energy transfer (FRET) based lipid mixing assay confirmed that fusion was enhanced, though the efficiency was lower than depletant induced fusion. This is significant because it shows that lipid-only synthetic liposomes, without non-lipidic components such as fusogenic peptides, fuse with EVs under physiologically relevant temperature and pH conditions. Differential interference contrast (DIC) and fluorescence microscopy reveal the clustering of mixtures of EVs and NLs, and EVs alone, in acidic but not neutral pH conditions, corresponding with conditions which enhanced fusion. These findings support the hypothesis that intracellular content release from EVs in the early to late endocytic environment is a function of protein-mediated clustering interactions and a lipidic component. Further, this study provides a novel method to enhance fusion of EVs and synthetic liposomes which is expected to preserve EV membrane proteins and functionality towards a therapeutic EV-liposome hybrid drug delivery vehicle for nanomedicine applications.

The Multivalent Cationic Lipid MVL5 Significantly Enhances the Solubility of Paclitaxel in Cationic Lipid Nanoparticle Membranes and Improves Cytotoxic Efficacy

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Cationic liposomes (CLs) with chain-melted, or fluid, membranes are promising nanocarriers (30-200 nm) of paclitaxel (PTX) and other hydrophobic drugs for cancer chemotherapy, with CL formulations (e.g. EndoTAG-1) showing success in preclinical and late-stage clinical trials. However, endosomal entrapment, limited PTX membrane solubility, and preferential tumor accumulation remain barriers to the success of CL carriers in clinical applications. Prior work has shown that the incorporation of the cone-shaped poly(ethylene glycol)-lipid (PEG-lipid) to CLs drives a transition to sterically stabilized, high-curvature micelles, or nanodiscs, with diameters of ≈15 to ≈35 nm in a fraction of the particles. These PTX loaded PEGylated CLs and nanodisccs showed enhanced cellular uptake *in vitro* as well as extended circulation half-life, significantly higher tumor penetration, and increased proapoptotic activity compared to bare CLs when tested on solid breast cancer tumor models in vivo. Recently, we made the remarkable discovery that formulations which incorporate the multivalent cationic lipid MVL5 (+5e) at 50 mol % form nanoparticle populations comprised almost entirely of nanodiscs. Here we demonstrate that the incorporation of MVL5 into lipid nanoparticle formulations improves the solubility or PTX in their membrane by nearly threefold and improves the cytotoxic efficacy of PTX-loaded vesicles compared to reference CLs modeled on the EndoTAG-1 formulation currently in clinical trials. Cell viability assays revealed that the cytotoxic efficacy of PTX loaded nanoparticles containing 50 mol % MVL5 is further improved by PEGylation. Finally, fluorescent microscopy imaging and automated image analysis show that the cellular uptake of fluorescently labeled nanoparticles containing MVL5 and reference CLs are improved by PEGylation. PEGylated cationic lipid nanoparticles containing MVL5 therefore represent a very promising hydrophobic cancer drug delivery vehicle for nanomedicine applications.

A Library of Custom PEG-Lipids Reveals a Double-PEG-Lipid with Drastically Enhanced Paclitaxel Solubility and Human Cancer Cell Cytotoxicity When Used in Fluid Micellar Nanoparticles

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Paclitaxel (PTX) is one of the most widely utilized chemotherapeutics globally.¹ However, the extremely poor water solubility of PTX necessitates a carrier for systemic delivery. Fluid lipid PTX nanocarriers (with lipid tails in the chain-melted state) show promise as PTX delivery vectors, but remain limited by the solubility of PTX within their membranes. To improve pharmacokinetics, membrane surfaces are typically coated with polyethylene glycol (PEG).² Recent work has demonstrated the generation of a population of micelles within fluid lipid formulations containing a 2kDa PEG-lipid at a 10 mol% ratio.³ Driven by the positive curvature of the PEG-lipid, these micelle-containing formulations were found to exhibit significantly higher uptake in cancer cells, cytotoxicity, and in vivo antitumor efficacy compared to formulations containing solely liposomes.³ Here, we describe the custom synthesis of a library of micelle-inducing PEG-lipids, and describe the effects of PEG chain length, chain branching (single- or double-PEG-lipid), and cationic charge on PTX solubility and cytotoxicity. We examined low (10 mol%) and high (100-x mol%, where x=PTX mol%) PEG-lipid formulations. Remarkably, all formulations containing the custom PEGlipids had improved PTX solubility over unPEGylated formulations and commercially available DOPE-5k. PTX solubility was highest in micellar formulations with a high content of a neutral lipid with a head group of two 2kDa PEG chains $(2k_2)$, which solubilized 13 mol% PTX for up to 24 h. The pancreatic cancer cell line PC3 exhibited higher sensitivity to formulations with high PEG-lipid content. The most potent formulations were prepared from $2k_2$ (IC50 = 14 nM). Our work suggests that formulations employing the custom PEG-lipids, particularly the double-PEG-lipid 2k₂, hold great promise as next-generation PTX delivery systems owing to their high PTX solubility, enhanced cell cytotoxicity, and potential for precision targeting by affixation of ligands to the PEG molecules.

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Scalable Synthesis of Tunable Surfactants Derived from α-Lipoic Acid Copolymers

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Polymeric surfactants, a class of amphiphilic polymers with hydrophilic and hydrophobic domains, are extensively used as surface-active agents as well as in various industrial processes. The hydrophobic-lipophilic balance, composition, and molecular weight of these surfactants are critical for achieving controlled polymeric architectures at interfaces, which are essential for superior surface activity. While living polymerization has been commonly employed to achieve such control, it is costly and labor-intensive due to the need for protection and deprotection of hydrophilic groups (e.g., sulfonic or carboxylic acids). Here, we introduce a novel approach to synthesize tunable polymeric surfactants with telechelic sulfonic acid (-SO₃H) groups via free-radical polymerization of bio-renewable, degradable lipoic acid derivatives and vinyl monomers. This process includes the reduction of disulfide bonds in the polymer backbone and subsequent oxidation of telechelic thiol polymers. Telechelic surfactants derived from 50 mol% lipoic acid derivative resulted in low-molecular-weight, water-soluble surfactants with excellent surface activity, including reduced surface and interfacial tension, and outstanding emulsifying properties. Conversely, using 30 mol% lipoic acid derivative produced high-molecular-weight, oil-soluble surfactants. This approach enables precise control over surfactant properties (e.g., hydrophobiclipophilic balance, composition, and molecular weight), facilitating the design of water-soluble to oil-soluble surfactants by simply varying the lipoic acid content, thereby expanding their potential applications in various fields of material science.

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Characterization of the Collapse Transition in a Peptoid Using Magnetic Tweezers

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The properties of biomaterials such as hydrogels can be tuned by incorporating force-sensitive

crosslinkers. Here, we investigate whether sequence defined peptoids can act as force responsive elements. Peptoids are biomimetic analogs to peptides and a candidate crosslinker material. In our experiments, we carry out elasticitv single-molecule precision measurements on collapsing peptoids using magnetic tweezers to gain insight into their conformational response to external forces. We will discuss peptoid linkage dynamics and the effect of peptoid sequence on chain conformation.



A. Experimental setup. Conformational response of self-attracting peptoids probed using magnetic tweezers. B. Peptoids predicted to exhibit similar conformational response to DNA hairpins. [1]

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Synthesis of Diblock Copolymer via Photo-Switchable RAFT Agent with Diarylethene

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Reversible addition - fragmentation chain transfer (RAFT) polymerization emerges as an effective tool for obtaining block copolymers which has multi component of monomers and RAFT agent structures have been devised according to the reactivity of each vinyl monomers. Vinyl monomers are broadly classified into conjugated monomers such as acrylate esters (more activated monomers, MAMs) and unconjugated monomers such as vinyl esters (less activated monomers, LAMs). Block copolymerization of MAMs and LAMs is difficult due to the different reactivity of each monomer, and limited examples have been reported¹.

In this study, a RAFT agent with pyridine as an electron acceptor connected to a dithiocarbamate via a photochromic diarylethene was synthesized and evaluated its polymerization behavior toward MAMs and LAMs. The produced RAFT agent has two isomers, a ring-opened (DEo) and a ring-closed (DEc) isomer derived from diarylethene, and each isomer can be switched by UV ($\lambda = 302$ nm) and Vis (530 nm) irradiation respectively. In DEo, the acceptor and RAFT agent are not electronically connected and thus exhibit controlled polymerization properties toward vinyl esters as dithiocarbamates, while in DEc, the electron density of the RAFT agent is reduced due to the electron-withdrawing nature of the acceptor via the π conjugated system of diarylethene and the acrylates showed controlled polymerization properties towards the acrylates.



Figure 1. Schematic illustration of photo-chromic behavior of DE RAFT agents and their controlled polymerization of VAc (LAM) and MA (MAM).

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Coarsening of Lipid Domains in Anisotropic Actin Network Elucidates Actin Polymer Nematics

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The growth of viscous droplets in 3D viscoelastic environments, observed in biological systems like biomolecular condensates, has motivated studies that demonstrate droplet growth abatement in these systems. Theoretical growth exponents are much lower than the 1/3 exponent expected for Ostwald ripening. In this study, we focus on the influence of elasticity on droplet growth specifically in 2D systems, such as cell membrane-cytoskeleton interfaces. We develop a phase-separating lipid membrane experimental system, where one phase is electrostatically coupled to a filamentous actin network which imparts elasticity. The competition between the thermodynamics of phase separation and the forces exerted by the network creates angular domains, such as triangles and tactoids, distinct from the bi-continuous structures observed in polymer viscoelastic mixtures. To support experimental observations, we develop a theoretical model where the actin network is treated as a liquid crystalline material, combining Cahn-Hilliard phase separation dynamics with a nematic order parameter. We demonstrate that, even in the absence of activity and hydrodynamics, the anisotropic nature of the network can significantly slow down coarsening. Furthermore, we show that the elasticity of the network can be modulated by actin density, and report growth exponents for varying densities. Through this study, we offer insights into the coupling of viscous and elastic phases in 2D biomaterials.

Mechanisms of Li Ion Transport in Zwitterionic Electrolytes from Molecular Dynamics Simulation

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Zwitterions possess both cationic and anionic groups covalently tethered within the same molecule, leading to unique properties. Recent studies have shown that polymer electrolytes with zwitterionic side chains exhibit remarkably high ionic conductivity and a high Li ion transference number, making them highly attractive for lithium-ion battery applications. ¹ However, the precise mechanisms that lead to these enhanced Li transport properties remain elusive. To provide deeper insight into the ion transport mechanism, we performed all-atom molecular dynamics simulations of amorphous zwitterion and Li salt mixtures. We explored the dynamic properties of the Li salts, the detailed local structures, and the interactions between Li ions and zwitterions/anions as a function of salt concentration. In this poster session, we will discuss how these atomic-level interactions and structures correlate with the overall ion transport properties and offer strategies for tuning electrolyte performance.



Figure 1. (a) The configuration of the simulation box (b) Chemical structures of zwitterion and Li salt

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A Photo-Caged Cyclopentadiene Resin for Digital Light Processing 3D Printing of Hydrogel Based on Rapid Diels-Alder Click Chemistry

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The potential of 3D printing technologies, particularly in the biomedical field, is being significantly enhanced by innovations in hydrogel chemistry combined with digital light processing (DLP) strategies.1 DLP offers unique advantages, especially for producing complex structures like cellladen tissues. However, traditional DLP techniques predominantly utilize radical photopolymerization of acrylate monomers, which can pose challenges for biological applications where the generation of radicals can adversely affect cell viability and alter proteins through unintended side reactions.² To address these limitations, we have explored Diels-Alder (DA) cycloadditions due to their high selectivity and compatibility with biological systems. Diels-Alder (DA) cycloadditions are preeminent click reactions, unlike other common click chemistries that rely on toxic additives. Inspired by the high reactivity of cyclopentadiene (Cp) for DA click reactions, we have recently reported the development of photo-caged Cp derivatives that enable efficient bioconjugation and control of polymer click reactions without the need for radicals.³ Herein, we utilized this photo-caged Cp strategy for the development of novel photo-resins for DLP printing of hydrogel materials that are formed by rapid gelation via the DA click reaction between Cp and maleimide. As a result, the photo-resin rapidly formed hydrogel networks on irradiation with light, through an additive and radical-free step-growth gelation process. Photo-rheology studies on the gelation of the resin revealed that the resin has an efficient photo-curability. Additionally, we have shown that the resin is suitable for post-functionalization of the 3D-printed hydrogels, showcasing the potential of photo-caged click chemistry for accessing next-generation 3D-printed materials. This development paves the way for next-generation 3D-printed biomaterials that are not only effective for various applications but also safe for biological systems, ultimately enhancing the functionality and integration of printed tissues and devices in the biomedical landscape.

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Compatibilization of Polystyrene and Polyolefins via Electrostatic Interactions

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Prior work has shown that small numbers of ionic interactions can be used for the compatibilization of immiscible polymer blends.^{1,2,3} This study aims to test the universality of this compatibilization strategy by blending polymers that exhibit various physical states (e.g., amorphous/semi-

crystalline, high/low glass transition temperatures). To achieve this, commercially available polybutadiene (PBD) was functionalized with various ratios of base groups and subsequently hydrogenated to yield polyethylene (PE) with the same degree of charge density. PBD and PE were then separately blended with polystyrene (PS) containing a low amount of sulfonic acid groups. We have demonstrated that incorporating ionic groups as low as 1 mol% leads to improved optical and mechanical properties upon blending. The blend processing routes were optimized, as properties can vary depending on the processing method. Furthermore, blending PBD with functionalized, recycled commercial PS resulted in improved material toughness. Blending PE with PS enhanced the overall durability of the final material, while the crystallinity of the final blend strongly depended on the relative charge of the blend components.



Enhanced properties of PBD/PS and PE/PS ionic blends.

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Ionic Crosslinking and its Influence on the Properties of Self-Doped Conjugated Polyelectrolytes

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CPE-K is a water-processable donor-acceptor conjugated polyelectrolyte with high electronic conductivity, due to its self-doping properties. However, its high solubility in water requires cross-linking to stabilize films for aqueous device applications. Despite its importance, the influence of crosslinking on CPE-K's properties remains unexplored. In this study, we employed divalent ionic cross-linkers (Mg²⁺, Ca²⁺, Sr²⁺, Ba²⁺) as an alternative to conventional covalent crosslinkers to enhance the stability of CPE-K films. Our results reveal that ionic cross-linking also improves the aqueous stability of CPE-K films while allowing for the characterization of their mechanical, morphological, and electrochemical properties. Notably, among the cross-linkers tested, Ba²⁺-cross-linked films exhibited the least swelling in



Figure 1. Swelling percentage of different ionic cross-linked CPE-K films in aqueous system.

water due to stronger electrostatic interactions with sulfonate groups. These strong interactions, however, resulted in the lowest ionic conductivity. While previous studies have examined donor-acceptor moieties, molecular weight, and alkyl side chain effects, the role of multivalent counterions has remained unexplored due to challenges in cross-linking and precipitation. This study addresses this gap, offering new insights into how multivalent cations impact the functional properties of CPE-K. These findings highlight the potential of ionic cross-linking as a versatile strategy to stabilize conjugated polyelectrolytes and optimize their performance for device applications.

Coupled High-speed Infrared Imaging and Multiphysics Modeling to Predict Three-Dimensional Thermal Characteristics during Selective Laser Melting

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The microstructures and hence mechanical properties of laser based additively manufactured metals are known to be sensitive to the thermal gradients and solidification velocity at the melt pool solid-liquid interface [1-6]. However, prediction of transient three-dimensional (3D) melt pool thermal characteristics during the solidification process remains elusive. Our unique approach couples high-speed infrared (IR) imaging at ~15000 fps, of the melt pool surface, with 3D multiphysics simulation to predict the sub surface transient temperature distribution and solidification conditions during selective laser melting of MAR-M247. Briefly, first, we capture the melt pool surface radiation using high speed IR imaging and convert it to melt pool surface temperature using a Planck's law-based custom calibration. Then, we import the experimentally obtained, spatio-temporally varying, melt pool top surface temperature as a boundary condition to a COMSOL model. Based on the experimentally obtained top surface temperature, the COMSOL model solves the 3D sub surface temperature distribution in and around the melt pool. Importantly, the coupled COMSOL model concurrently solves for the complex melt pool multiphysics which involves conduction, phase change (solid⇔liquid) and thermal Marangoni induced flow inside the melt pool. We validate the predicted melt pool cross section, depth and width with the ex-situ scanning electron microscopy (SEM). Further, we quantify the much-needed local 3D solidification conditions such as: thermal gradient, solidification velocity and solidification direction at the melt pool solid-liquid interface. Using ex-situ SEM, we validate that, during solidification, the grain growth direction closely follows the 3D thermal gradient direction at the S-L interface, as predicted by the coupled model. Further, based on these local solidification conditions, crucial to microstructure growth, the model suggests a reduction in cell width of the solidified microstructure, as the laser scan speed is increased from 500 mm/s to 1000 mm/s for 200 W laser power. The cell width predictions from the coupled model are validated by a comparative cell width analysis of ex-situ SEM for 200 W – 500 mm/s and 200 W – 1000 mm/s laser scanning parameters. We believe the multi-dimensional and data rich outcomes of our methodology can readily be coupled with machine learning and present a platform that can viably be translated to commercial settings.

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Hydrations Dynamics Near Polyelectrolyte and Zwitterionic Surfaces

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The dynamics of local water molecules surrounding charge-containing polymers regulate surfacesolute interactions throughout the system and dictate the efficacy of these materials in water separation membranes and protective coatings. However, the dynamics of water near chemical surfaces varies greatly from the behavior of bulk water and is experimentally difficult to resolve with most methods. In this study, Overhauser Dynamic Nuclear Polarization (ODNP) relaxometry

is utilized to measure hydration dynamics within 15 Å of nitroxide spin labels distributed across polymer surfaces and correlated to bulk properties. Specifically, the dynamics around linear poly(acrylic acid) (PAA) chains and zwitterion-functionated water filtration membranes are explored. PAA is a superabsorbent polymer which absorbs up to 1000 times its mass in water and is expected to promote meaningful water-polymer interactions. In PAA solutions, measurements of the relaxivity parameter k_{σ} , which directly correlates to the local water diffusivity, suggest that water dynamics fluctuate between similar to bulk water to slower than other hydrophilic polymer systems depending on polymer concentration and the ionic environment. This lends direct insights into the nature



The dynamics of water in the vicinity of PAA chains vary drastically based on polymer concentration and ionic environment

of hydration ordering around the PAA surface, with deprotonated carboxylic acid groups disturbing the local hydration layer and preventing hydrogen bonding while protonated carboxylic acid groups directly incorporate into water's hydrogen bonding network. In zwitterionic membrane systems, local hydration dynamics can be directly correlated to macroscopic properties such as permeability and water uptake to formulate a molecular understanding of the water and ion transport.

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Engineering Soft, Elastic, and Conductive Polymers for Stretchable Electronics Using Ionic Compatibilization

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Designing materials that are soft, elastic, and conductive—a complement of properties that are useful in a number of applications such as bio-interfacing—remains a major challenge due to the high stiffness of conventional conductive materials. For all-polymer systems, this problem is compounded by the general immiscibility of elastomeric and conducting polymers, resulting in inhomogeneous mixing and poor properties. Here,



Soft, Elastic, Conductive Complex

electrostatic interactions are shown to be an effective strategy to compatibilize distinct polymer chemistries and backbone architectures, resulting in homogeneous and multifunctional polymer complexes that are soft, elastic, and highly conductive. An anionic conjugated polyelectrolyte (CPE) based on polythiophene was blended with a cationic bottlebrush polyelectrolyte (BPE). The CPE provided electrical conductivity, while the BPE helped to control the mechanical properties. Strong electrostatic attractions between oppositely charged side chains of the CPE and BPE suppressed phase separation and the polymers formed a nearly homogeneous charged complex despite marked differences in their chemistry and architecture. Upon drying of the solvent, the ionic groups act as dynamic crosslinks and the resulting material behaved as a viscoelastic and reprocessable solid. Once doped with a strong acid, this composite had an electrical conductivity of up to 0.3 S/cm while maintaining a low tensile modulus (0.2 MPa). These findings highlight the potential of designing advanced materials with processing and performance advantages through the use of electrostatic interactions to compatibilize polymers.

Structures and Interactions in Lipid-RNA Complexes by Optical Microscopy

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Lipid-drug conjugates (LDCs) and/or lipid nanoparticles are widely used as a drug delivery system. Lipids are a suitable vector for drugs as they improve the stability and half-life of the inherently unstable compounds, while also allowing entry into the cell [1]. LDCs can surpass other challenges of a traditional route of drug delivery — lipid nanoparticles can be specifically tailored to deliver the drug to a particular tissue in a patient's body, while having minimal side effects due to its small size [2]. mRNA-based therapeutics hit a milestone when COVID-19 vaccines became available. mRNA delivery is faster than DNA delivery as mRNA does not need to enter the nucleus and can be translated directly from the cytoplasm. A range of therapeutic applications is possible with mRNA, including but not limited to viral vaccines, protein replacement therapies, cancer immunotherapies, etc [3,4,5,6].

Here, we focus on characterizing cationic liposome-RNA (CL-RNA) complexes using differential-interference-contrast (DIC) and fluorescence microscopy. Specifically, we look at how the lipid/RNA molar charge ratio at distinct salt concentrations and pH values affect the structures of the CL-RNA complexes. The studies are designed to enable an understanding of the nature of the electrostatic interactions in lipid membrane-RNA systems.

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Bottom-Up Coarse-Grained Modeling of Sequence-Specific Polymers

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Molecular modeling offers direct insight into conformational landscapes, enhancing our understanding of sequence-structure relationships. In this work, we use sequence-specific peptoids as a platform for developing design rules for relating chemical sequence to polymer conformation. Polypeptoids are particularly useful in this context due to their lack of backbone hydrogen bonding, isolating the effect of sidechain chemical sequence on polymer chain shape. Moreover, they are routinely synthesized at gram scale, sequence-specifically, with hundreds of different side chain functionalities, allowing for detailed experimental investigation and validation. However, polypeptoid simulations encounter major sampling challenges due to the long-time scales associated with conformational transitions, which has greatly limited fundamental studies on broader peptoid chain shape effects and self-assembly behaviors. Recently, our studies of small polypeptoid systems with all-atom advanced sampling molecular dynamics revealed the local and global structure of short chains in response to their sequence patterning to be in excellent agreement with experiments. In this work, we developed a bottom-up coarse-grained peptoid model, which allows access to longer and multiple peptoid systems. With this simulation workflow we study the effect of sequence on broader chain shape effects. Moreover, this CG workflow enables the development of models that can be readily transformed into field-theoretic representations, facilitating the exploration of larger length scales and phase behavior.

Microwave-Assisted Synthesis of Layered Sodium-Ion Battery Cathodes: Controlling Sodium Content for Enhanced Electrochemical Performance

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Lithium-ion batteries have proved crucial in facilitating the expansion of renewable energy into our everyday lives. There are, however, significant sustainability limitations and ethical concerns associated with the sourcing lithium and cobalt feedstocks. Sodium-ion batteries attract interest as promising alternative energy storage devices, owing to the high natural abundance of sodium and the potential to achieve high energy densities in systems that do not rely on cobalt or nickel redox.

One concern with sodium layered oxide materials is the existence of multiple crystalline phases, as controlled by sodium content. 6-coordinate sodium can occupy either octahedral or prismatic sites between the metal oxide layers, which affects anion packing and symmetry. As such, the electrochemical behavior of the material is fundamentally altered. One such example is P2-layered $Na_{2/3}[Mn_{1/2}Fe_{1/2}]O_2$, which despite having a lower theoretical capacity, is capable of achieving 190 mAh g⁻¹ of reversible capacity upon discharge, while O3-layered $Na[Mn_{1/2}Fe_{1/2}]O_2$ only achieves only 110 mAh g⁻¹ despite having higher initial sodium content.¹ Careful control of elemental composition, and corresponding stricture, is therefore key to unlocking advanced electrodes for sodium ion batteries.

The volatility of sodium at high temperatures makes targeting specific compositions, and therefore specific sodium coordination environments, difficult using conventional sub-solidus ceramic synthesis techniques. These techniques require extended periods of time at elevated temperatures approaching 1000 °C. We propose a rapid microwave-assisted synthetic route to prepare sodium electrodes. Microwave-based preparation methods for solid-state synthesis have garnered interest for its facile setup, fast reaction rates, and cost-effectiveness. The short timescale and homogeneous heating facilitated by microwave synthesis allows us to precisely control sodium content, elemental composition and crystalline structure. We use advanced diffraction techniques and element specific analysis to probe the effect of composition and structure on the electrochemical performance of these materials. We propose these methods as a cost-effective and efficient route to synthesis of layered sodium electrodes.

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Tunable Photo-Fading Liquid Crystal Elastomers Enabled by Broad Range Polarity of Donor Acceptor Stenhouse Adducts

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Since their discovery in 1981 by Finkelmann and others (ref), liquid crystal elastomers (LCEs) have emerged as a very promising class of soft materials which can harness different stimuli such as electricity, magnetism, heat and/or light (in this work). The use of photochromic entity inside LCEs enables them to generate responses like color change, photomechanical contraction, bending and photothermal heat generation under light stimulation. Incorporation of a negative photochrome such as Donor Acceptor Stenhouse Adducts (DASA) in LCE has opened avenues to tune spectroscopic, photothermal and optomechanical properties. This was achieved by varying the acceptor strength of the carbon acid in DASA which creates a polarity spectrum from neutral to zwitterionic DASAs. This work is an attempt to predict DASA properties in LCEs based on the structure-property relationship in solution phase and provide a comprehensive overview of how DASA behaves in material in general. The solution phase parameter that helped bridging the behavior in the solution and in the materials is solvatochromic slope. It is shown how such a simply determinable parameter can hold the power to predict photo-fading behavior of DASAs in LCEs and the rate at which the photo-fading occurs. Additionally, optomechanical characterization revealed tunability in photoinduced strain generation in correlation with photothermal heating. The tunable color and photo-bending response were further demonstrated using various series patterns of varying DASA-LCEs.

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Using Quantitative FTIR to Elucidate Hydration Kinetics of Small Molecules

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To meet society's growing materials and energy demands, energy efficient separation technologies are necessary. Thermal separation processes such as distillation and evaporation, account for 8% of the energy consumed within the United States. Membrane-based separation technologies have the potential to reduce energy consumption by up to 90%. However, membrane performance is challenged by the accumulation of undesired material on the surface (i.e., fouling). Current fouling management relies on altering process conditions and physical/chemical cleaning; these techniques limit the deposition and remove fouled species, respectively, but they do not address the root cause. To design antifouling membranes, research has shifted towards functionalizing surfaces with small molecules that repel foulants (e.g., zwitterions and polyethylene oxide). While zwitterion and polyethylene oxide functionalized surfaces are effective at mitigating fouling on the macroscale, the specific molecular-scale interactions that inhibit fouling remain unclear. Current literature suggests that the fouling resistance arises from (1) strong interactions with the water molecules in the first hydration shell or (2) rapid hydration dynamics. Understanding the complex relationship requires techniques capable of probing both the kinetics and thermodynamics of water exchange at the binding site.

This poster highlights preliminary work whereby quantitative FTIR is used to elucidate the hydration kinetics of small molecules. We highlight the design of an FTIR apparatus that carefully controls atmospheric water content to probe the binding of water molecules in the first hydration shell. Tracking the kinetics of H₂O/D₂O exchange enables the regression of both kinetic and thermodynamic parameters. The methods described here lay the groundwork to characterize zwitterions with subtle changes in structure (e.g., tether length, diffuseness of the cation). Ultimately, the data generated will be compared to macroscale fouling experiments to understand how molecular scale interactions translate to antifouling performance. Additionally, by understanding the relationship between the thermodynamics and kinetics of water in the hydration shell, this work will generate design principles that can be used to reverse engineer antifouling chemistries.

Resolving Thermal Gradients and Solidification Velocities During Laser Melting of a Refractory Alloy

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Metal additive manufacturing (AM) processes, such as powder bed fusion (PBF), can yield highvalue parts with unique geometries and features, substantially reducing costs and enhancing performance. However, these processes are highly sensitive to thermal effects, and thermal information can impact the quality of the printed microstructures. In this study, we present a novel methodology for converting high-speed IR images of the melt pools during laser melting of a Nbbased C103 alloy into temperature maps. This method integrates radiation over the wavelength range of the IR detector and assigns the liquidus temperature to the melt pool boundary, eliminating the need for sophisticated X-ray imaging. We further develop a technique to resolve temperature gradients, cooling rates, melt pool dimensions, and solidification velocities with high temporal and spatial resolution. Notably, during solidification, the thermal data indicate that a decreasing thermal gradient and increasing solidification velocity from the edge to the center of the melt pool can lead to a transition from epitaxial to equiaxed grain morphology in the alloy. These findings highlight the critical role of detailed thermal characterization in understanding and optimizing microstructural outcomes in additive manufacturing.

The thermal measurement and analysis part of this work is supported by the National Science Foundation through the Materials Research Science and Engineering Center (MRSEC) at UC Santa Barbara: NSF DMR–2308708 (Seed). The laser melting experimental setup and mate- rials characterization are based upon work supported by the Department of Energy, National Nuclear Security Administration under Award Number(s) DE-NA0004152.

Chemical Stability and Interfacial Transport in Dual Electrolyte Solid-State **Batteries**

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Dual solid electrolyte architectures offer a path towards energy-dense all-solid-state batteries by combining an electrolyte stable against a high voltage cathode with one stable against a low voltage (e.g., metallic) anode. However, the interface between possible solid electrolyte pairs must be better

understood, both in terms of reactivity and ionic transport, to identify optimal chemistries that allow stable long-term cycling. In this work, we examine the compatibility of chloride and sulfide electrolytes for use in bilayer solid-state batteries, whereby the chloride is the catholyte.¹ Prior studies have shown that certain chloride and sulfide electrolyte chemistries are incompatible, including Li₃InCl₆ and argyrodite Li₆PS₅Cl.² Here, we choose to examine the stability of Li₂ZrCl₆ against two commonly used sulfide electrolytes, Figure 1. Contour plots of a series of Li₆PS₅Cl and Li₃PS₄. Through heat treatments of the electrolyte mixtures, we introduce reaction temperature as a proxy for chemical compatibility under battery ramp from 25°C up to 300°C followed by a operating conditions and characterize electrolyte temperature hold at 300°C.





degradation using a combination of solid-state nuclear magnetic resonance, X-ray diffraction, Raman spectroscopy, and X-ray photoelectron spectroscopy. While neither pairing is thermodynamically stable according to first principles calculations, synchrotron X-ray diffraction with in-situ heating shows that Li₂ZrCl₆-Li₆PS₅Cl is stable up to higher temperatures compared to Li₂ZrCl₆-Li₃PS₄ (280°C vs. 90°C, see Figure 1), and this pairing also leads to stable cycling in an allsolid-state cell. Using electrochemical impedance spectroscopy, we show that the activation barriers for conduction in Li₂ZrCl₆-Li₆PS₅Cl bilayer pellets decrease after a 110°C heat treatment at a pressure of 70 MPa for 24 hours, indicating that the system is suitable for hot calendaring.

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Non-Ideal Mixing Drives Complex Micellization Morphology and Phase Behavior of Mixed Nonionic Surfactants

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Mixtures of surfactants are frequently used to modify the self-assembly, interfacial, and temperature properties of surfactant and emulsion formulations. In many cases, property data are interpreted assuming that chemically homologous co-surfactants completely mix at the molecular scale, often with ideal mixing thermodynamics. However, limited studies with co-surfactant mixtures involving large differences in spontaneous curvature lead to a number of non-ideal phenomena including non monotonic mixture phase behavior and complex assembled structures in solutions and emulsions. To better elucidate the molecular origins of this behavior we report combined structural, thermodynamic, and chemical characterization in model mixed ethoxylated alkane (CiEj) co surfactants in aqueous solutions (water/surfactant) and oil-in-water microemulsions. Phase behavior and calorimetric studies in these mixtures exhibit a significant non-monotonic dependence of critical temperatures and micellization thermodynamics that indicate non-ideal mixing in co surfactants with disparate spontaneous curvature (e.g., $C_{12}E_5/C_4E_1$) relative to geometrically similar co-surfactant pairs (e.g., C12E5/C12E6). Using a combination of viscometry, dynamic light scattering (DLS), contrast-variation small angle neutron scattering (CV SANS), and 2D nuclear magnetic resonance (NMR) measurements to resolve micelle morphology and intermolecular interactions, we show that this behavior corresponds with significant temperature-dependent differences in solvation between the mixed surfactants and their pure component counterparts. Ultimately, we hypothesize that differential solvation structures between co-surfactants in the mixed state provide a potential explanation for all the observed non-ideal behavior, and we test this hypothesis against molecular dynamics and field-theoretic simulations.

Enhancing Thermal Stability of Organic Photodetectors with Polymer Acceptors

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Organic Photodetectors (OPDs) are essential in diverse modern applications, including digital imaging, biological sensing, optical communication and remote control. However, the low stability under thermal stress is one of the obstacles that are hindering the commercialization of OPD, and this is caused by the morphology change of the active layer, which is composed of a blend of a donor and an acceptor. Herein, we replaced the commonly used small-molecule acceptor, Y6, with three polymer acceptors, namely PF5-Y5, PYTS-C2, and PY2TS-C2, based on the structure of Y6, to suppress the morphology change thus enhancing the thermal stability of OPDs. Blended with the donor PBDB-T, all OPDs show reasonable dark current density (J_d) and external quantum efficiency (EQE). After thermal annealing, the OPD based on PF5-Y5 showed slight EQE drop under -2 V, and the OPDs based on PY₂TS-C₂ and Y6 showed severe J_d increase. The grazing-incidence wide-angle X-ray scattering (GIWAXS) result manifests phase separation after annealing in the active layer based on Y6, and the resonant soft X-ray scattering (RSoXS) results indicates mixing feature for PF5-Y5 system. We further found that the EQE drop in the PF5-Y5 based OPD is due to the electron mobility drop after annealing. Besides, the J_d increase in the PY2TS-C2 and Y6 based OPDs is probably due to the emerging deeper trap states after thermal annealing. By annealing the active layer only and depositing the top electrode afterward, we found that the J_d increase in the PY2TS-C2 OPD mainly comes the diffusion of the top electrode into the active layer, while the phase separation in the active layer also plays a role in the PY2TS-C2 system.

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Selective Phase Stabilization in Microwave-Prepared NaSICON Solid Electrolytes Through Potassium Ion Exchange

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Sodium solid-state batteries offer a promising alternative to lithium-ion batteries, leveraging the abundance of sodium paired with the increased safety and high energy density of ceramic electrolytes. The solid electrolyte material NaSICON is generally prepared through solid-state reaction consisting of heat treatment for several hours in a furnace. Since the energy required for heat treatment drives the cost of ceramic oxide membranes,¹ developing low energy intensity synthesis methods is necessary to commercialize solid electrolytes. In this study, NaSICON is prepared through microwave-assisted solid-state synthesis and densified through rapid induction hot pressing. Microwave-assisted solid-state reaction pathways can reach high temperatures of up to 1500°C in a short period of time² through direct heating of the precursor mixture, allowing for rapid reaction times and energy efficiency.

Using the combination of microwave synthesis and rapid induction hot pressing, densified samples with high conductivities of 6-7 mS cm⁻¹ were achieved. Arrhenius analysis of variable temperature electrochemical impedance spectroscopy data gives a bulk activation energy of 0.25 eV with a total activation energy of 0.29 eV. Rietveld refinement of synchrotron x-ray diffraction data shows a mixture of monoclinic and rhombohedral NaSICON structures with minor secondary phases of monoclinic zirconia and β '-quartz (SiO₂).

NaSICON is a solid solution series with the composition $Na_{1+x}Zr_2(SiO_4)_x(PO_4)_{3-x}$. The composition $Na_{3,4}Zr_2Si_{2,4}P_{0,6}O_{12}$ has been previously shown to exhibit the maximum conductivity above 5 mS cm^{-1,3} While the end members $NaZr_2(PO_4)_3$ and $Na_4Zr_2(SiO_4)_3$ crystallize in the rhombohedral R -3c (no. 167) space group, $Na_{3,4}Zr_2Si_{2,4}P_{0,6}O_{12}$ crystallizes in a mixture of the monoclinic C 2/c (no. 15) and rhombohedral R -3c (no. 167) space groups, with monoclinic as the primary phase. In this work, synthesized NaSICON is immersed in potassium chloride solution resulting in an ion exchange between sodium and the larger potassium ion, which selectively stabilizes the rhombohedral phase with a 4% increase in the c lattice parameter. Room temperature stabilization of the rhombohedral phase, which is generally stable above 200°C,³ has potential implications on sodium conductivity due to an increase in the size of the sodium diffusion channel within the crystal structure.

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High-Throughput Characterization of Protein-Protein Interactions and Assembly Using Differential Dynamic Microscopy for Material Formulations

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Protein-based materials have become a crucial part of the bioengineering industry, with applications ranging from pharmaceuticals to bioelectronics. Rational design and development of these materials requires characterization of the impact that protein-protein interactions and assembly structures have on the resultant material properties across a wide formulation space. However, conventional biophysical characterization techniques often require homogeneous or dilute samples, invasive sample preparation, or have large material requirements, making it unfeasible to conduct such characterization on proteins with expensive and time-consuming synthesis processes. By contrast, recent studies have demonstrated how high-speed video microscopy of protein solutions can be combined with differential dynamic microscopy (DDM) analysis to extract the hydrodynamic size, virial coefficient, and phase behavior associated with protein-protein interactions akin to conventional light scattering. By relying solely on concentration fluctuations of species below the diffraction limit, protein DDM can be performed on a range of systems without the need for complex labeling or super resolution microscopy to resolve protein structure and dynamics. Here, we demonstrate how protein DDM can be adapted for high-throughput measurements and analysis, providing insight into the fundamental interactions driving assembly of polyclonal Immunoglobulin G. The results show promise for developing intensified, high-throughput measurements of scarce biomolecular materials to aid discovery and design of natural and engineered protein assemblies.

In situ observation of thermally-activated and localized Li leaching from lithiated graphite

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Temperature is known to significantly impact Li-ion battery performance and safety.¹ While previous studies have sought to understand the effects of homogeneous, low or high temperatures, there is a much more limited body of work exploring the effects that non-uniform temperatures such as temperature hot spots have on Li-ion batteries.^{2,3} We have utilized in situ micro-Raman spectroscopy and optical microscopy to simultaneously induce and probe the effect of a microscale temperature hotspot on a graphite electrode. While graphite is known to be prone to Li plating during lithiation at low temperatures and/or high C-rates, our results reveal that localized temperature heterogeneity induced by the micro-Raman laser can cause Li to leach out from LiC₆ and LiC₁₂ in the absence of an applied current. Raman spectra and optical micrographs of the graphite are complemented by thermal simulations to estimate the temperature distribution induced by the Raman laser on the graphite electrode. The leached Li is found to be localized to the temperature hotspot and shown to be dependent on the laser power density (E_{laser}) with higher E_{laser} inducing larger temperature variation across the electrode and more severe Li leaching from LiC₆ and LiC₁₂. A mechanism whereby localized temperature heterogeneity induced by the laser induces heterogeneity in the degree of lithiation across the graphite electrode is proposed to explain the localized Li leaching from LiC_6 and LiC_{12} . Such results have important implications for the safety and performance of batteries as mild temperature heterogeneity in the absence of current has not been considered as a condition which could lead to Li formation on the surface of graphite via leaching.

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Enzymatic Regulation of the Phase Behavior of DNA Nanostars

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Inspired by the discovery of liquid-like condensates and their functions in living cells, recent theoretical studies have predicted various intriguing behaviors for phase-separating biomolecules subject to biochemical reactions, such as suppression of coarsening, droplet differentiation, and long-range spatial ordering. However, corresponding experimental studies remain limited.

Here, we introduce a simple experimental model using DNA nanostars that involve enzymaticallycontrolled dimerization chemical reactions: non-phase-separating monomers exhibit a uniform fluid state, and transform into phase-separating dimers through an enzymatic reaction. The reaction kinetics and phase separation patterns can be characterized by gel electrophoresis and confocal microscopy observation, respectively. We discuss how phase behaviors^{1,2,3} such as droplet formation, degradation and wetting affinity (Fig.1), change as a function of forward and backward reaction rates.



Fig.1 Dynamic control of the wetting affinity of nanostar liquid droplets through a ligase/restriction enzyme reaction cycle. Sequential images show snapshots of nanostar droplets at various time points: t = 2, 4, 8 and 16 hours. Initially, two distinct, non-interacting droplets, colored yellow and pink, begin to adhere and progressively increase their contact line over time. The side length of each image is approximately 400 µm.

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Low-Temperature Properties of Bismuth Double Perovskites

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Lone pair halide double perovskites have garnered significant interest as non-toxic alternatives to lead-based perovskites for active optoelectronic devices. While extensive research has been conducted on the structure and optical properties of bismuth double perovskites at room temperature, studies exploring their behavior at low temperatures are scarce. Utilizing single-crystal/powder X-ray diffraction and Raman spectroscopy, we have identified phase transitions in several bismuth-based double perovskites, including Cs₂AgBiBr₆, Cs₂AgBiCl₆, and Cs₂NaBiCl₆, at low temperatures.

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Bandwidth as a Determinant of Metallicity in Oxides

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Oxides are a ubiquitous class of materials exhibiting a wide range of structures and properties with applications from battery electrodes to high-temperature superconductors. The diversity of oxide phenomena can be attributed to the nature of metal—oxygen bonds that can span ionic and covalent interactions. In this work, we focus on oxides featuring metallic conduction to highlight the connections between these bonding environments, the atomic-level structure, and the electronic structure. While frameworks for understanding metallicity in oxides have been developed, we identify the bandwidth of states near the Fermi level as an overlooked criterion. Through a survey of oxide metals, we point out the requisite condition of dispersive bands (large bandwidth) to obtain metallic conduction. We extend the discussion of the critical role of bandwidth to flat bands which can be associated with correlated physics and unconventional superconductivity. While we center on oxides in this work, these concepts are applicable across crystalline inorganic materials.



Examples of oxides encompassing the range of electronic bandwidths. LK-99 features phosphate groups resulting in localized electrons and, therefore, flat bands. ReO₃ exhibits a three-dimensional network of covalent interaction allowing for high electron mobility and dispersive bands.

High Throughput Search for Photostrictive Materials based on a Thermodynamic Descriptor

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Photostriction is a phenomenon that can potentially improve the precision of light-driven actuation, the sensitivity of photodetection, and the efficiency of optical energy harvesting. However, known materials with significant photostriction are limited, and effective guidelines to discover new photostrictive materials are lacking. In this study, we perform a high-throughput computational search for new photostrictive materials based on simple thermodynamic descriptors, namely the band gap pressure and stress coefficients. Using the Δ -SCF method based on the density functional theory, we establish that these descriptors can accurately predict intrinsic photostriction in a wide range of materials. Subsequently, we screen over 4770 stable semiconductors with a band gap below 2 eV from the Materials Project database to search for strongly photostrictive materials. This search identifies Te₂I as the most promising candidate, with photostriction along out-of-plane direction exceeding 8 × 10⁻⁵ with a moderate photocarrier concentration of 10¹⁸ cm⁻³. Furthermore, we provide a detailed analysis of factors contributing to

strong photostriction, including bulk moduli and band-edge orbital interactions. Our results provide physical insights into photostriction of materials demonstrate the effectiveness of using simple descriptors in high-throughput searches for new functional materials.

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Disentangling the Impact of Chemical Doping and Electrostatic Complexation on Optoelectronic Properties of Organic Mixed Ion-Electron Conductors

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Mixed ion-electron conducting polymers have garnered significant attention in recent years for applications in batteries, bioelectronics, optoelectronic and electrochemical devices since mixed conductors afford the transport of ionic and electronic species as well optical and mechanical tunability. Contradictory morphological rules for electron and ion conduction create performance challenges, making the optimization of conduction of both species of particular interest and importance for device applications. Our group's previous work has shown that the electrostatic compatibilization of mixed conducting conjugated polyelectrolytes (CPE's) with electrically insulating polyelectrolytes can produce complex, mixed conducting films with reasonable electronic conductivity ($10^{-3} - 10$ S/cm) yet without the crystallinity or structure traditionally needed. The complex films have even outperformed films made solely out of the same CPE used for the complexation.^{1,2,3} In addition, we have shown that the complexes outperform a traditional battery binder in ionic conductivity and battery cell performance.^{1,3} To better understand why we see this difference in electronic performance between the CPE and complex films and, therefore, to develop new insights into how to design mixed conductors for improved electronic performance, we have looked at a model system in which we compare P3HT-based CPE (poly{3-[6'-(Nmethylimidazolium)hexyl]thiophene Br⁻} or P₃HT-Im⁺Br⁻) and a complex (of the same CPE and poly(sodium 4-styrenesulfonate) or P3HT-Im⁺PSS⁻). Upon electronic doping, a process required for most organic conductors to achieve application-relevant properties, the addition of extrinsic charge carriers should alter the structure and performance of the films. In this way, we see can directly see how the complexation of the CPE to yield a more processable, highly concentrated film impacts the mixed conduction performance and structure of the films under controlled doping, which should provide insight into the effects and challenges of electronic doping processes. This work focuses on understanding the behavior of electronic charge transport in mixed conductors to inform and improve device performance, from batteries to active device layers.

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Electric-Field-Induced Thermal Switching in a Bulk Ferroelectric Material at Room Temperature

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Active thermal management requires advances in thermal switching materials, whose thermal conductivity responds to external stimuli. The electric field, as one of the most convenient and effective methods, has shown great potential in tuning the thermal conductivity of ferroelectric

materials, particularly in transistors where large built-in electric fields are present. While previous studies on electric-field-induced ferroelectric thermal switching have primarily focused on thin films, bulk materials, which are more promising for practical applications, have received comparatively less attention. In this study, we experimentally demonstrate the significant impact of domain structure on the thermal conductivity of the ferroelectric barium titanate (BaTiO₃) at room temperature, which can be controlled by an electric field to realize thermal switching. By utilizing customized steady-state methods and TDTR measurement, the in-plane and out-of-plane



thermal conductivity was systematically studied under electric fields up to $\pm 10 \text{ kV/cm}$ at room temperature. Furthermore, we investigated the aging effect on their thermal switching properties and found that aging enhances the variation in thermal conductivity by nearly 100%. This research highlights the crucial role of aging effects in ferroelectric materials for improving their thermal switching ratios, paving the way for designing novel electric-field-induced thermal switching materials. This work is based on research supported by the U.S. Office of Naval Research under the award number No0014-22-1-2262.

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