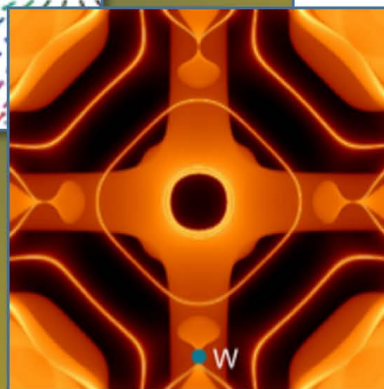
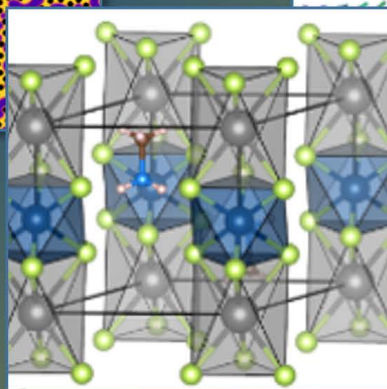
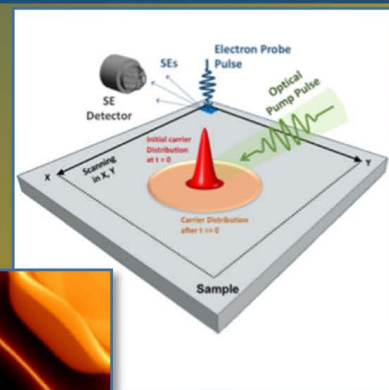
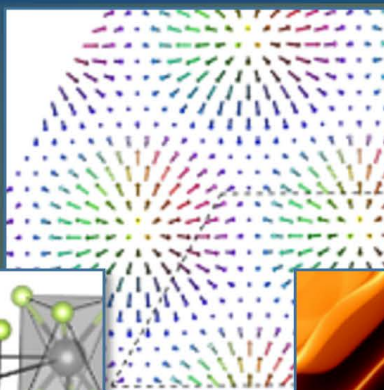
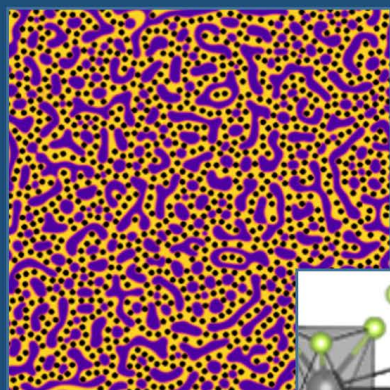


NSF Materials Research Science and Engineering Center [DMR 1720256]



Materials Research Outreach Program

Wednesday January 29th and Thursday January 30st 2020
Corwin Pavilion, UC Santa Barbara
Schedule and Poster Abstracts



Materials Research Outreach Symposium
Wednesday, Jan 29 to Thursday, Jan 30, 2020, Corwin Pavilion, UC Santa Barbara

About the MROP

Initiated in 1999 under the leadership of the late Professor Edward Kramer to annually showcase MRL research to our Industrial and Venture partners, the Materials Research Outreach Program has evolved into so much more. In addition to providing a wonderful opportunity to interface with our corporate colleagues — including, and perhaps especially, local start-ups — the MROP has emerged as the principal occasion to hear about and share UC Santa Barbara research in the broad Materials arena.

The MROP has traditionally encouraged many new faculty members from a cross-section of UC Santa Barbara departments to showcase their research vision, leading to the nucleation of numerous collaborations. Academics, particularly from neighboring campuses, are also invited. Finally, the MROP has become an integral part of the undergraduate and graduate education, and post-doctoral experience of literally hundreds of students and fellows from Science and Engineering Departments on this campus.

No matter which category best fits you, please feel welcome to attend the 2020 MROP, and thank you for your continued support. We hope you enjoy the MROP as much as we enjoy organizing it.

Materials Research Outreach Symposium
Wednesday, Jan 29 to Thursday, Jan 30, 2020, Corwin Pavilion, UC Santa Barbara

Session 1, Wednesday Morning, January 29, 2020, Corwin Pavilion

8:45 am	Opening remarks by Dean Rod Alferness	
9:00 am	<i>Stephen Wilson</i>	Quantum Foundry at UC Santa Barbara
9:30 am	<i>Angela Pitenis</i>	Resilience via Compliance: Designing Soft Materials for Biomedicine
10:00 am	<i>Refreshment Break</i>	
10:30 am	<i>Neil Treat, Google</i>	Materials Science at the Moonshot Factory
11:00 am	<i>Matt Helgeson</i>	Data-Driven Approaches for Processing Flowing Soft Materials
11:30 am	<i>Chris Spadaccini, Lawrence Livermore National Laboratory</i>	Additive Manufacturing and Architected Materials: New Processes and Materials
12:00 pm	<i>Lunch</i>	

Session 2, Wednesday Afternoon, January 29, 2020, Corwin Pavilion

1:30 pm	<i>Matt Tirrell, University of Chicago</i>	Polyelectrolytes in Multivalent Ionic Media: New Physics and New Materials
2:00 pm	<i>Rubayn Goh</i>	Adaptive Survival Capsules for Developing Shark Embryos
2:30 pm	<i>Refreshment Break</i>	
3:00 pm	<i>Cecilia Leal, UIUC</i>	Block-Copolymer – Phospholipid Alloys
3:30 pm	Cheetham Lecture: <i>Tim Lodge, University of Minnesota</i>	Bicontinuous Structures in Charged Polymer Materials
4:30 pm	<i>Posters and Reception</i>	

Materials Research Outreach Symposium
Wednesday, Jan 29 to Thursday, Jan 30, 2020, Corwin Pavilion, UC Santa Barbara

Session 3, Thursday Morning, January 30, 2020, Corwin Pavilion

9:00 am	<i>Molleigh Preefer</i>	High Electronic and Ionic Conductivity in Lithium Battery Electrodes
9:30 am	<i>Kim See, Caltech</i>	One is the Loneliest Number: Multivalent Cations and Multielectron Processes for Next-Generation Batteries
10:00 am	<i>Refreshment Break</i>	
10:30 am	<i>Galan Moody</i>	Quantum Light Generation with 2D Materials: Progress, Challenges, and Opportunities
11:00 am	<i>Yolita Eggeler</i>	Microscopy of Engineered Magnetic Materials
11:30 am	<i>Brian Haidet</i>	Epitaxial Integration of Novel Chalcogenide Materials on to a III-V Platform for Electronics and Photonics
12:00 pm	<i>Lunch</i>	

Session 4, Thursday Afternoon, January 30, 2018, Corwin Pavilion

1:30 pm	<i>Cristina Marchetti</i>	Topological Defects in Active Nematics
2:00 pm	<i>Nick Scherck</i>	Integrated Particle and Field-Theoretic Simulations: A Multiscale Approach to Complex Soft Matter Formulations
2:30 pm	<i>Max Robb, Caltech</i>	Force-Activated Covalent Bond Transformations via Polymer Mechanochemistry
3:00 pm	<i>Refreshment Break</i>	
3:30 pm	<i>Vojtech Vlcek</i>	New Theoretical Approaches to Electronic Excitations at the Nanoscale
4:00 pm	<i>Mahdi Abu-Omar</i>	SperoSet Technology for Renewable and Recyclable Composites
4:30 pm	<i>Yon Visell</i>	Emerging Material Technologies for Haptics and Robotics

Program Conclusion

Dr. Abu-Omar has 20 plus years of experience in R&D management and technology development. Mahdi is the Founder and CEO of Spero Renewables, a clean tech company that provides cost-effective and renewables substitutes to petrochemicals. Mahdi holds the Duncan and Suzanne Mellichamp Chair in Green Chemistry at the University of California, Santa Barbara (UCSB). His research accomplishments include selective conversion of biomass lignin to biophenols and the creation of renewable plastics based on lignin. He has authored more than 200 original research articles in peer-reviewed scientific journals, supervised more than 40 Ph.D. students, and held faculty appointments at Purdue University and UCLA. Mahdi was elected Fellow of the American Association for Advancement of Science (AAAS) in 2012 and was a Senior Fulbright Fellow at the Weismann Institute in 2008. Dr. Abu-Omar completed his Ph.D. from Iowa State University and a postdoc from Caltech.



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Yolita M. Eggeler joined the Materials Department at UC Santa Barbara in October 2018 as a postdoctoral scholar following her PhD degree from the Materials Science and Engineering Department at the Friedrich-Alexander University (FAU) in Germany. She is a recipient of the Feodor-Lynen postdoctoral research fellowship sponsored by the German Humboldt Foundation. At UCSB she is a member of the research groups of Prof. Gianola and Prof. Pollock, and her research is an integral part of the collaborative NSF Materials Research Science and Engineering Center (MRSEC). Specifically, she is interested in the evolution of micro- and nanostructures and their effect on structural and functional properties. She investigates engineered two-phase materials, which find applications as either load bearing blade materials in state of the art jet engines or in next-generation technologies such as magnetic refrigeration and spintronic devices. To better understand the interplay between microstructure evolution and properties she uses analytical electron microscopy techniques. In her spare free time, she tries to catch lobsters but has so far been unsuccessful.



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Rubayn Goh received his B.Eng in Materials Engineering from Nanyang Technological University in 2014 and spent a year in the Molecular Engineering Lab led by Dr Sydney Brenner at A*STAR before joining the Ph.D program in the Materials Department at UCSB. His current work involves developing an understanding of the fundamentals behind multi-functional and tough biological materials under the co-advisement of Professors Herbert Waite and Rachel Segalman.



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Brian Haidet earned Bachelors in Physics and Materials Science and Engineering from North Carolina State University in 2016, working on metal-semiconductor junctions in the AlGa_N alloy system under Ramon Collazo and Zlatko Sitar. Currently, he is a PhD Candidate and NSF Graduate Research Fellowship recipient with the Materials Department at UCSB in the Mukherjee Group. His current research focuses on heteroepitaxial MBE growth and characterization of IV-VI semiconductors. Outside the lab, Brian also runs a small YouTube channel based on science and making.



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Matt Helgeson is Associate Professor of Chemical Engineering at UCSB, and is Co-Leader of IRG₃: Resilient Multi-phase Soft Materials in the MRL. Prof. Helgeson's research focuses on the engineering of multi-phase fluids with controlled mesoscale structure, particularly through the use of flow and thermal processing. Recent examples include the development of nanostructured emulsions for templating multi-phase nanoparticles and soft solids, as well as engineering complex flows to optimize anisotropic structure in colloidal materials. To support this research, the Helgeson group develops custom fluidic devices for *in situ* characterization of microstructure and rheology during flow using microscopy and scattering methods. Prof. Helgeson's research has been recognized with a number of recent awards including the Unilever Award from the American Chemical Society and early career awards from the National Science Foundation and Department of Energy.



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Cecilia Leal is an Associate Professor and Racheff Faculty Scholar of Materials Science and Engineering at the University of Illinois at Urbana-Champaign (UIUC). She is also affiliated with the Materials Research Laboratory and the Beckman Institute. Cecilia received a M.S. in Industrial Chemistry from the University of Coimbra in Portugal and a PhD in Physical Chemistry from the University of Lund in Sweden. Cecilia was a Swedish Research Council postdoctoral fellow in Materials Science at the University of California in Santa Barbara before she started her appointment at UIUC in 2012. Her research interests lie at the intersection of materials science and physical chemistry with a focus on soft materials relevant in biology. Cecilia is the recipient of the 2019 UIUC Office of Provost Distinguished Promotion Award, the 2018 UIUC College of Engineering Dean's Award for Excellence in Research, the 2016 NSF CAREER Award, and the 2016 NIH Director's New Innovator Award.



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Tim Lodge graduated from Harvard in 1975 with a B.A. cum laude in Applied Mathematics. He completed his PhD in Chemistry at the University of Wisconsin in 1980, and then spent 20 months as a National Research Council Postdoctoral Fellow at NIST. Since 1982 he has been on the Chemistry faculty at Minnesota, and in 1995 he also became a Professor of Chemical Engineering & Materials Science. In 2013 he was named a Regents Professor, the University's highest academic rank. He has been recognized with the American Physical Society (APS) Polymer Physics Prize (2004), the International Scientist Award from the Society of Polymer Science, Japan, (2009), the 2010 Prize in Polymer Chemistry from the American Chemical Society (ACS), and the Hermann Mark Award (2015) and the Paul Flory Education Award (2018) of the ACS Division of Polymer Chemistry. He has been elected to Fellowship in the American Association for the Advancement of Science, the APS, the ACS, and the Neutron Scattering Society of America. In 2016 he was elected to the American Academy of Arts and Sciences. From 2001–2017 Tim served as the Editor-in-Chief of the ACS journal *Macromolecules*. In 2011 he became the founding Editor for *ACS Macro Letters*. He has served as Chair of the Division of Polymer Physics, APS (1997–8), and as Chair of the Gordon Research Conferences on *Colloidal, Macromolecular and Polyelectrolyte Solutions* (1998) and *Polymer Physics* (2000). Since 2005 he has been Director of the NSF-supported Materials Research Science & Engineering Center at Minnesota. He has authored or co-authored over 450 papers in the field of polymer science, and advised or co-advised over 80 PhD students. His research interests center on the structure and dynamics of polymer liquids, including solutions, melts, blends, and block copolymers, with particular emphases on self-assembling systems using rheological, scattering and microscopy techniques.



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M. Cristina Marchetti is a Professor of Physics at the University of California Santa Barbara. She was educated in Italy at the University of Pavia, earned her Ph.D. in the U.S. at the University of Florida, and joined the faculty at UC Santa Barbara in 2018, after thirty years on the faculty at Syracuse University. Marchetti is a versatile theoretical physicist who has worked on a broad range of problems in condensed matter physics, including supercooled fluids, superconductors and driven disordered systems. Currently, she is interested in understanding the emergent behavior of "active matter". The name was coined to describe large collections of living creatures that exhibit organized behaviors on scales much larger than that of the individuals. Examples range from the flocking of birds to the sorting and organization of cells in morphogenesis, and include synthetic analogues, such as active colloids and engineered microswimmers. Marchetti is currently co-lead editor of the *Annual Reviews of Condensed Matter Physics* and of *Physical Review X*. She is a Fellow of the American Physical Society and of the American Association for the Advancement of Science, and a member of the American Academy of Arts and Sciences and of the US National Academy of Sciences. In 2019 she was awarded the inaugural Leo P. Kadanoff prize by the American Physical Society "For original contributions to equilibrium and non-equilibrium statistical mechanics, including profound work on equilibrium and driven vortex systems, and fundamental research and leadership in the growing field of active matter."



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Galan Moody is an Assistant Professor in the Electrical and Computer Engineering Department at UCSB (July 2019). Prior to moving to Santa Barbara, he was a Research Scientist (2015-2019) at the National Institute of Standards and Technology (NIST) in Boulder, Colorado, a postdoctoral fellow at NIST (2013-2015), and a postdoctoral associate at the University of Texas Austin (2013). He received his PhD in Physics (2013) and his BSc in Engineering Physics (2008) from the University of Colorado-Boulder. His research focuses on fabricating and characterizing integrated quantum photonic devices and quantum materials relevant for quantum information processing, communications, and metrology, including 2D materials, semiconductor quantum dots, and hybrid quantum systems. His recent honors and awards include a National Research Council Fellowship (2013), the Superlattices, Nanostructures, and Nanodevices Young Scientist Award (2018), NIST's Innovations in Measurement Science Award (2019), and an AFOSR Young Investigator award (2020).



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Angela Pitenis is an assistant professor in the Materials Department of the University of California, Santa Barbara. She earned her PhD from the University of Florida, and her research interests are focused on energy dissipation mechanisms at soft, biological, and bio-inspired material interfaces.



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Molleigh Preefer is a PhD candidate in the Department of Chemistry and Biochemistry and the materials research laboratory at UC Santa Barbara. She received her B.A. in Chemistry from Columbia University and did research with Professor Colin Nuckolls on synthesizing aromatic carbon-based molecules for solar cell applications. At UC Santa Barbara she works with Professor Ram Seshadri synthesizing and characterizing a range of materials for battery applications, including Li-S, all-solid-state, and Li-ion technologies. She combines electrochemistry, synchrotron techniques, Raman spectroscopy, and X-ray photoelectron spectroscopy to understand the underlying redox mechanisms in battery materials.



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Max Robb was born and raised in Colorado and obtained his B.S. in Chemistry from the Colorado School of Mines. After graduating in 2009, Max carried out his Ph.D. studies in the laboratories of Prof. Craig J. Hawker at the University of California, Santa Barbara. His doctoral research focused broadly on the synthesis of functional organic materials and was recognized by the American Chemical Society with the 2016 Henkel Award for Outstanding Graduate Research in Polymer Chemistry. Max conducted postdoctoral research with Prof. Jeffrey S. Moore at the University of Illinois, Urbana-Champaign as a Beckman Institute Postdoctoral Fellow prior to joining the Division of Chemistry and Chemical Engineering at Caltech as an Assistant Professor in September 2017. Research in the Robb group seeks to advance the fundamental understanding of mechanical force transduction at the molecular level and develop strategies to create force-responsive functional materials.



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Kimberly See is an Assistant Professor of Chemistry in the Chemistry and Chemical Engineering Division at Caltech. She was born and raised in Colorado and received her B.S. in Chemistry from the Colorado School of Mines in 2009 where she worked with Drs. John Turner and Todd Deutsch at the National Renewable Energy Laboratory on photoelectrochemical water splitting. Following a year at the University of Colorado working with Prof. Gordana Dukovic on zinc oxide nanoparticle synthesis and a year in industry at NuSil Technology working on high refractive index silicones, Kim pursued her PhD in Chemistry at the University of California, Santa Barbara. She worked with Profs. Ram Seshadri and Galen Stucky on next-generation batteries and received her Ph.D. in 2014. Kim was then awarded the St. Elmo Brady Future Faculty Postdoctoral Fellowship at the University of Illinois at Urbana-Champaign and worked with Prof. Andrew Gewirth in the Department of Chemistry until the fall of 2017. Her postdoctoral work focused on the solvation structure of active cations in electrolyte solutions in Li-S and Mg batteries. Now, her group at Caltech is interested in new chemistry for next-generation energy storage with a focus on Earth abundant, inexpensive materials. She focuses on the electrochemistry associated with multivalent and multielectron processes.



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Nick Sherck joined the Ph.D. program in the Chemical Engineering Department at UC Santa Barbara in the Fall of 2016 following his bachelor's degree from the Chemical Engineering Department at Purdue University. At Purdue, he worked on sequence-controlled polymer synthesis in the laboratory of Professor You-Yeon Won. At UC Santa Barbara, Nick is co-advised by both Professors Glenn Fredrickson and Scott Shell. His initial work was the study of colloidal interactions in polymer solutions, using field-theoretic and molecular dynamics simulations. Currently, he is working on a computational framework to allow for the study of industrially relevant soft matter formulations. Specifically, his work involves the coupling of atomistic to field-theoretic simulations using relative entropy coarse-graining.



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Christopher M. Spadaccini, Ph.D., is currently the Director of the Additive Manufacturing Initiative at the Lawrence Livermore National Laboratory (LLNL) as well as the leader of the Center for Engineered Materials and Manufacturing. He has been working in advanced additive manufacturing process development and architected materials for the last decade and has over 60 journal publications, four book chapters, ~75 invited presentations, and ~35 patents awarded or pending. Dr. Spadaccini founded several new fabrication laboratories at LLNL for process development focused on micro and nano-scale features and mixed material printing. He received his B.S., M.S., and Ph.D. degrees from the Department of Aeronautics and Astronautics at the Massachusetts Institute of Technology (MIT) in 1997, 1999, and 2004 respectively and has been a member of the LLNL technical staff for over 15 years. He has also been a lecturer in the Chemical, Materials, and Biomedical Engineering Department at the San Jose State University where he taught graduate courses in heat, mass, and momentum transfer. He is currently also an adjunct faculty member at the University of California, Davis in the Chemical Engineering Department.



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Matthew Tirrell's research has been in the fields of polymer interfaces, dynamics, fluid phase behavior and nanomedicine. He is particularly known for his work on polymer brushes, surface force measurement, peptide amphiphiles and polyelectrolyte complex phase behavior. In 2011, Matthew Tirrell was appointed as the founding Pritzker Director and Dean of the Faculty of the Institute for Molecular Engineering and established the first University of Chicago engineering program, which he continues to oversee (now the Pritzker School of Molecular Engineering). Professor Tirrell simultaneously served as Deputy Laboratory Director for Science (September 2015 - April 2018) and Chief Research Officer (January 2017 - March 2018) at Argonne National Laboratory. Immediately prior to joining the University of Chicago, he was the Arnold and Barbara Silverman Professor and Chair of Bioengineering at the University of California, Berkeley, with additional appointments in chemical engineering and materials science & engineering, as well as a Faculty Scientist appointment at the Lawrence Berkeley National Laboratory. Dr. Tirrell completed ten years as Dean of Engineering at the University of California, Santa Barbara on June 30, 2009. From 1977 to 1999, he was on the faculty of Chemical Engineering and Materials Science at the University of Minnesota, where he served as department head from 1994 to 1999. Tirrell received a B.S. in Chemical Engineering at Northwestern University in 1973 and a Ph.D. in 1977 in Polymer Science from the University of Massachusetts. He has co-authored about 400 papers and one book, has supervised about 100 Ph.D. students and 50 postdoctoral researchers. Professor Tirrell is a member of the National Academy of Engineering, the National Academy of Sciences, the American Academy of Arts & Sciences and the Indian National Academy of Engineering, and is a Fellow of the American Institute of Medical and Biological Engineers, the AAAS, and the American Physical Society.



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Neil Treat is a Material Scientist in the early pipeline at X, formerly Google X, which invents and launches moonshot technologies that could make the world a radically better place. He received his PhD in Materials from UC Santa Barbara, aimed at understanding the phase separation in bulk heterojunctions of semiconducting polymers and fullerenes for photovoltaics. Before X, he was a Marie Curie Fellow at Imperial College London and Senior Material Scientist in the Platform Technologies Group in Imerys.



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Yon Visell directs the RE Touch Laboratory at the University of California, Santa Barbara, www.re-touch-lab.com, which is investigating haptics, wearable technologies, and soft robotics. Visell is Associate Professor in the Media Arts & Technology Program, Department of Electrical and Computer Engineering, and Department of Mechanical Engineering (by courtesy). He is affiliated with the California NanoSystems Institute and the UCSB Center for Polymers and Organic Solids. He received the Ph.D. in Electrical and Computer Engineering from McGill University, was a postdoctoral scholar at Sorbonne University, and served on the faculty at Drexel University. Visell has published more than 70 scientific works, including two edited volumes on haptics and VR, and spent more than five years working in industry. He has three times received and 11 times been nominated for awards at leading academic conferences. Visell received a Google Faculty Research Award in 2016, a Hellman Family Foundation Faculty Fellowship in 2017, and a US National Science Foundation CAREER award in 2018. Dr. Visell is General Co-Chair of IEEE Haptics Symposium, the longest running conference in the field.



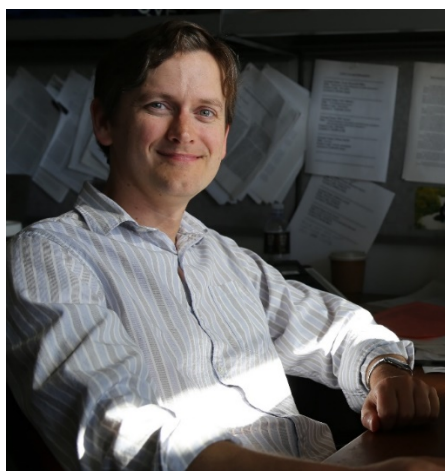
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Dr. Vlcek and his group develop new theoretical approaches on the boundary of several disciplines with a strong focus on condensed matter theory. Their goal is to understand the electronic excitations in quantum materials and the dynamics of electron-electron interactions using advanced many-body diagrammatic methods. In quantum materials, the quantum interactions extend over nanometer scales, which were often deemed untractable by conventional theoretical approaches. The group of Dr. Vlcek is pioneering new methods that break the current computational limitations and apply advanced quantum many-body theory to complex nanoscale systems. Dr. Vlcek received his Ph.D. in 2016 jointly from The Hebrew University of Jerusalem (Israel) and University of Bayreuth (Germany), where he studied in chemistry and physics departments. His Ph.D. was sponsored by the Minerva Fellowship of the Max Planck Society. From 2016 till 2018, Dr. Vlcek continued as a postdoctoral researcher at UCLA in the Department of Chemistry and Biochemistry. He joined the faculty at UCSB in 2018. In 2019, Dr. Vlcek received an NSF CAREER Award for the development of a new generation of stochastic many-body methods.



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Prof. Stephen Wilson serves as an Associate Professor and the Associate Chair of the Materials Department at the University of California, Santa Barbara. After obtaining his Ph.D. from the Physics Department at University of Tennessee in 2007, he worked at Lawrence Berkeley National Laboratory as a postdoc prior to joining the faculty of the Physics Department at Boston College in 2010 as an Assistant Professor. After moving to UC Santa Barbara in 2014, he was appointed an Associate Director of the California Nanosystems Institute, and he now serves as a co-director of the recently established Quantum Foundry on campus. His research group focuses on the synthesis and exploration of novel quantum materials. Of particular interest is the study of electronic states and phase behaviors in quantum magnets and strongly spin-orbit coupled correlated electron systems.



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Nonsolvent Induced Phase Separation with Particles and Droplets

R. Alhasan^a and D. R. Tree^a

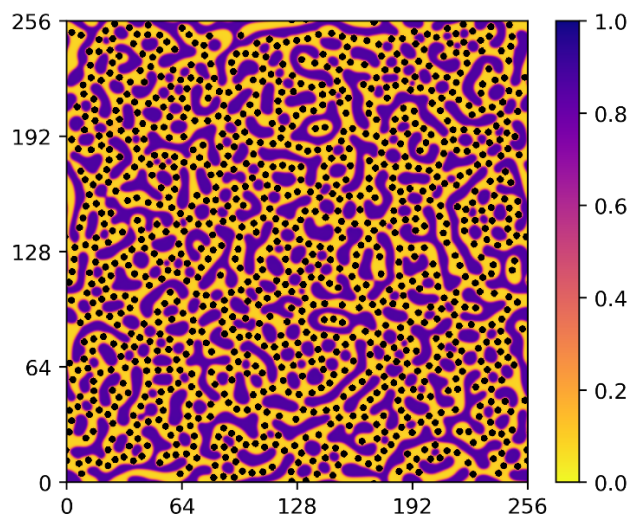
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The morphology of a polymeric structure that evolves in a nonsolvent induced phase separation (NIPS) remains vague and begs for a more quantitative approach. Motivated by previous work where we simulated the formation of polymer membranes via NIPS in a film geometry^{1,2}, we investigate the NIPS process in the presence of finite-sized droplets. We explore two different questions. First, we explore the NIPS process in a finite-sized droplet of polymer solution. Similar to the case for films, we find that three qualitatively different structures develop depending on the initial volume fraction of polymer in the solution. However, distinct from films we find that the Marangoni flow related to NIPS in droplets depends strongly on droplet size. To explain this effect, we estimate a Marangoni number (Ma) and show how it depends on both the size and concentration of droplets in our model. In addition, we critically examine previous reports of the existence of a critical Marangoni number indicating the onset of flow. Second, we investigate the spinodal decomposition phenomena in the presence of solid colloidal particles with different wetting properties as shown in Figure 1. We find that the wetting behavior of the particles has a significant impact on the bicontinuous structure resulting from the phase transition.

We acknowledge the financial support from Brigham Young University and computational resources from the BYU Office of Research Computing.

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A bicontinuous morphology after phase separation in the presence of particles with selective wetting properties.

Determination of the Structure-Property Relationship at the Hydrogel Surface

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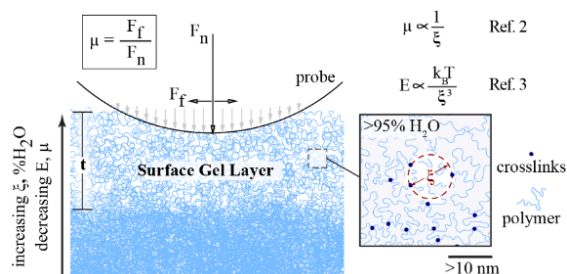
Soft aqueous gels are commonly utilized to model biological materials due to their ability to mimic the mechanical and tribological properties of these soft tissues and form hierarchical structures.¹ Poly(acrylamide) (PAAm) is a highly characterized hydrogel that is often utilized for this purpose because the average spacing between crosslinked chains, the mesh size (ζ), can easily be tuned by controlling polymer and crosslinker concentrations.² While the relationship between mesh size and elastic modulus (E) of hydrogels has been widely known since de Gennes' seminal work,³ the effect of changing mesh size on other properties, such as the coefficient of friction (μ), has not been clearly established. Recent studies have suggested that the mesh size of the hydrogel surface layer may be drastically different from the bulk depending on the polymerization conditions.^{4,5}

This work focuses on the characterization of PAAm hydrogels with varying concentrations to gain fundamental understanding of the interplay between processing, structure, and mechanical property. By inhibiting the polymerization process, hydrogels were cast with a gradient in crosslinking density through the thickness of the sample ("surface gradient hydrogels") and compared to hydrogels with comparatively uniform crosslinking density. Confocal microscopy was utilized to characterize the surface gradient while the elastic modulus was obtained through atomic force microscopy. A custom-built microtribometer was used to determine that the surface gradient hydrogels have lower coefficients of friction than those with uniform crosslinking density.

This work was supported by the MRSEC Program of the National Science Foundation under Award No. DMR 1720256.

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Schematic of the architecture of a surface gradient hydrogel with important scaling relationships listed. Inset: The mesh size, the average spacing between crosslinks, is indicated by the red circle.

Development of Ultrafast SEM: a tool to visualize spatio-temporal evolution of photocarriers in materials

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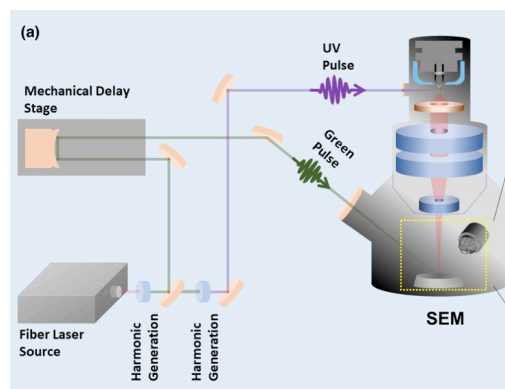
Ultrafast lasers have enabled studies probing the dynamics of charge carriers in materials in the femtosecond to nanosecond regime. However, probing the spatial dynamics of carriers in these ultrafast time domains has remained challenging. In this work, we describe the development of Scanning Ultrafast Electron Microscopy (SUEM), a novel tool that enables the study of spatio-temporal evolution of excited carriers in materials on fs time scales and μm to nm length scales¹⁻³. In SUEM, a conventional SEM is coupled to an ultrafast laser with pulse width ~ 200 fs. The heating current to the SEM's electron source is reduced until no emission is observed. A beam from the fs laser source is tightly focused onto the tip of the electron gun, generating electron pulses. A second beam is focused onto a sample in the SEM chamber and excites electrons in the material. Areas with increased concentrations of photoexcited electrons manifest as bright contrast in produced images. The time delay between the optical pump pulse and the electron probe pulse can be varied, allowing for the generation of snapshot images at different time points during a dynamical process of interest.

SUEM has been used to probe photocarrier dynamics in semiconductors such as $\text{Si}^{1,4,5}$, GaAs^1 , and CdSe^1 , has characterized a super-diffuse transport regime in Si^4 , and been used to image and characterize transport at interfaces like a Si p-n junction.⁶ Here, we report some preliminary results in heavily doped n- and p-type Si and discuss future capabilities.

The research reported in this work has in part been supported by the DOE Office of Science and the US Army Research Office.

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Schematic of SUEM experimental setup showing fs laser coupling with SEM.

Evolution of magnetic properties and magnetic entropy change in $\text{Co}_{1-x}\text{Mn}_x\text{Cr}_2\text{O}_4$

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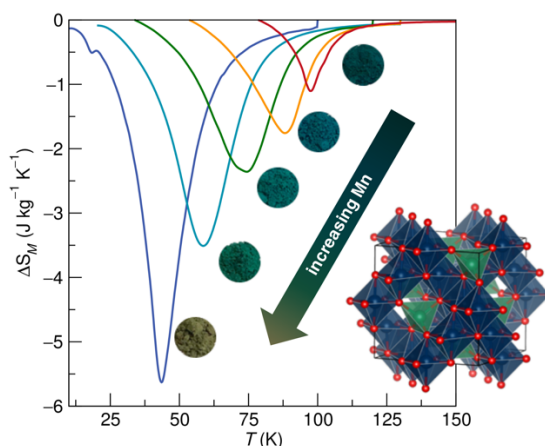
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Magnetic refrigeration and magnetic waste-heat recovery are accomplished with materials displaying the magnetocaloric effect – a reversible temperature change upon application of a magnetic field. In recent decades, this technology has been proposed as an environmentally friendly alternative to traditional vapor-compression technology, obviating chlorofluorocarbon refrigerants, and potentially capable of greater efficiency.¹ A figure of merit for magnetocalorics is the magnetic entropy change, ΔS_M . It has been proposed that magnetostructural coupling affects the magnitude of ΔS_M , and that compounds with potentially large ΔS_M can be screened for through the use of a computational proxy called the magnetic deformation (Σ_M).² This proxy has identified many compounds as magnetocaloric candidates, several of which are in the spinel structure type (AB_2O_4) with varying compositions and different values of Σ_M . Here, we investigate changes throughout an isomorphous solid solution in the spinel structure type by controlling the Co to Mn ratio in the tetrahedrally coordinated A site. Because trivalent Cr strongly prefers the octahedrally coordinated B site, this solid solution presents an opportunity to restrict site substitution to the tetrahedral site and understand how chemical identity and spin state in affect magnetostructural coupling and the magnetocaloric effect.

This work was supported by the National Science Foundation through DMR-SSMC 1710638. The research reported here made use of shared experimental facilities of the National Science Foundation (NSF) Materials Research Science and Engineering Center at UC Santa Barbara, DMR-1720256.

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ΔS_M maximum value and occurrence temperature is tunable by changing the Co to Mn ratio in the spinel structure.

End-to-end distance distributions of intrinsically disordered polypeptoids

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Sequence controlled polypeptoids provide a valuable platform for systematic study of molecular level changes in polymer patterning and chemistry; however, limitations in understanding of sequence effects on polymer conformation and challenges in modeling polypeptoids persist. In this work, distributions of polypeptoid end-to-end distances calculated from molecular dynamics (MD) simulations are compared to those obtained experimentally in order to provide insight on sequence-conformation relationships and validate MD force fields. Two experimental methods, double electron electron resonance (DEER) spectroscopy and continuous-wave electron paramagnetic resonance (cw-EPR) lineshape analysis, are used to span a range of distance from about 1-6 nm. DEER determines a distribution of distances between spin labels placed at each end of a polymer chain, while an average end-to-end distance can be calculated from dipolar broadening observed by cw-EPR. Together, MD and EPR techniques provide a methodology for understanding the impact of polymer sequence and chemistry on polymer conformation as well as confidence in MD prediction of other properties, such as local hydration dynamics at polymer surfaces.

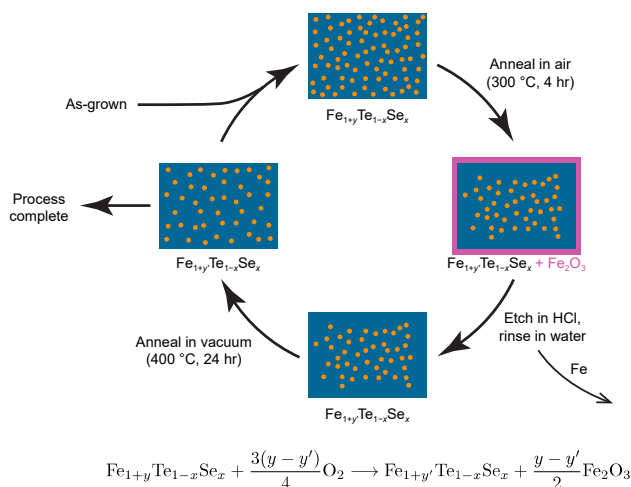
Bulk superconductivity in $\text{FeTe}_{1-x}\text{Se}_x$ via physicochemical pumping of excess iron

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The iron-based superconductor $\text{FeTe}_{1-x}\text{Se}_x$ has attracted considerable attention as a candidate topological superconductor owing to a unique combination of topological surface states and bulk high-temperature superconductivity.^{1,2} The superconducting properties of as-grown single crystals, however, are highly variable and synthesis dependent due to excess interstitial iron impurities incorporated during growth.³⁻⁶ Here we report a novel physicochemical process for pumping this interstitial iron out of the $\text{FeTe}_{1-x}\text{Se}_x$ matrix and achieving bulk superconductivity as shown in the figure to the right. Our method should have significant value for the synthesis of high-quality single crystals of $\text{FeTe}_{1-x}\text{Se}_x$ with large superconducting volume fractions.



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Probing complex coacervate droplet growth and size distribution using microfluidicsC. E. R. Edwards^a and M. E. Helgeson^a^aChemical Engineering Department
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Coacervation is implicated in a number of bioprocesses that result in high-function materials—e.g. extracellular matrix growth,^{1,2} mussel adhesive plaque formation,^{3,4} and transient recruitment of low-concentration enzymes via membraneless organelles^{5,6}—which synthetic systems cannot yet match. Mimicking these processes using synthetic polymers will open up new material designs, but requires understanding coacervate behavior out of equilibrium. Despite hints in the literature that processing parameters may determine whether aggregates or soluble complexes form from solutions of synthetic polyelectrolytes,⁹ the effect of mixing parameters has not been directly addressed. Prior measurements of complex-coacervate growth from salt solutions of synthetic polyelectrolytes use scattering after stopped-flow mixing (i.e. maximum turbulence only).^{7,8} Herein, a new microfluidics-based method to study coacervate growth kinetics enables control over mixing initiation and timescale that is not possible with stopped-flow. Additionally, sizing droplets by processing microscopy videos, rather than using scattering, permits measurement of the instantaneous size distribution and accurate sizing across the Mie scattering limit. To demonstrate these capabilities, charge-balanced coacervates from aqueous NaCl solutions of poly(allylamine hydrochloride) and poly(acrylic acid sodium salt) are imaged as they grow in laminar flow. Droplet size distribution and growth kinetics are characterized as salt and polymer concentration is varied. Comparisons to off-chip measurements of time-dependent turbidity and apparent phase under other mixing conditions reveal that increased turbulence enhances transient aggregation.

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Modeling the formation of phase inversion membranes: effects of arrested mobility and thermal fluctuations

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Many polymer membranes are made by immersion of a polymer solution film in a nonsolvent bath: the mass transfer exchange between the nonsolvent from the bath and the solvent in the film induces phase separation of the film into a polymer-rich phase that becomes the membrane matrix and a polymer-poor phase that becomes the membrane pores. Microstructure formation of these membranes is still not fully understood due to the nature of the physical processes involved: the mass transfer induced phase separation, the coarsening of domains, and the vitrification of the polymer-rich phase that arrests membrane microstructure. In this work, we use phase-field models of the ternary polymer-nonsolvent-solvent system to solve the coupled convection-diffusion and momentum equations that describe membrane formation. We model the glass transition using contrasts in the viscosity and mobility of the polymer-rich and polymer-poor phases. We report how glassy dynamics, and the inclusion of thermal fluctuations, contribute to microstructure formation.

Probing nonequilibrium dynamics and structure of polymeric liquids using orthogonal superposition rheology

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Understanding how microstructural dynamics change in flow is critical for understanding and modeling the flow processing of soft materials and complex fluids. This is particularly important for entangled polymeric fluids, where entanglements produce nonlinear relaxation mechanisms that are significantly modified when polymers stretch and orient in flow, leading to various flow instabilities and complications in polymer processing. Here, we introduce orthogonal superposition (OSP) rheology as a powerful tool for studying the coupling of microstructural dynamics and nonlinear rheological response in polymeric liquids. By superposing a small oscillatory motion orthogonal to the direction of a steady shearing flow, OSP provides measurement of the frequency- and shear-rate-dependent nonlinear viscoelastic superposition moduli (storage and loss moduli, G' and G''), which are analogous to their linear viscoelastic counterparts that characterize equilibrium dynamics. Although the method was proposed more than half a century ago¹, recent instrumental advances have finally enabled sensitive OSP on commercially available rheometers², including a new acquisition in the MRL Polymer Characterization Facility.

Because OSP has only recently become experimentally available, very little is known about how to interpret the nonlinear viscoelastic results in the context of entangled polymer dynamics. To fill this gap, here we report the first OSP calculations using current state-of-the-art models for entangled polymers, *i.e.*, the Rolie-Poly Model for monodisperse polymers and the Rolie-Double-Poly Model for polydisperse polymers.^{3,4} These models account for the detailed nonlinear relaxation processes of entangled polymers including reptation, chain retraction and convective constraint release. Simulations of OSP enable direct quantification of how each relaxation mode contributes to the superposition moduli. We find that the superposition moduli are only sensitive to the material stress contributions arising from chain retraction and convective constraint release, providing an effective means of isolating their rheological signatures and, in principle, directly measuring the molecular parameters governing their magnitude. Studying orthogonal superposition computationally not only provides important comparison to future experiments, but also offers unprecedented sensitivity in testing models for nonlinear polymer processing.

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Controlling Dzyaloshinskii-Moriya interactions in the skyrmion hosts $\text{FePd}_{1-x}\text{Pt}_x\text{Mo}_3\text{N}$

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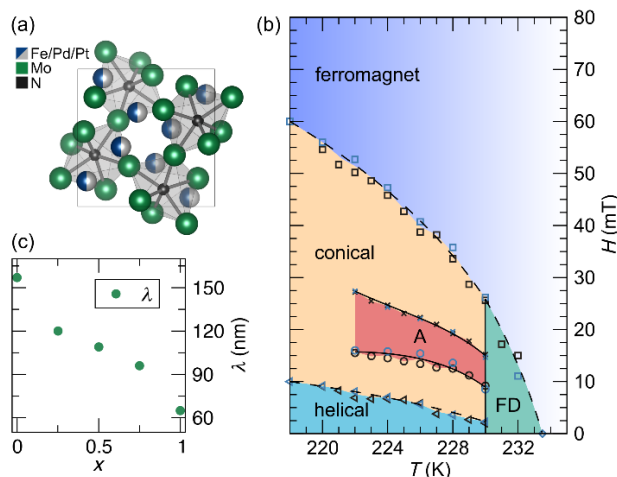
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Ferromagnets crystallizing in structures described by chiral cubic space groups, including compounds with the B20 or β -Mn structures, are known to host long-period chiral spin textures such as skyrmion lattices. These spin textures are stabilized by a competition between ferromagnetic exchange and antisymmetric Dzyaloshinskii-Moriya (DM) exchange, which is enhanced by the spin-orbit coupling associated with high-atomic-number elements. For real-world application, it is desirable to find materials that can host compact skyrmion lattices at readily accessible temperatures. Here, we report on the crystal chemistry and magnetic phase diagrams of a family of compounds with the filled β -Mn structure, $\text{FePd}_{1-x}\text{Pt}_x\text{Mo}_3\text{N}$ with T_C ranging from 175 K to 240 K. DC and AC magnetization measurements reveal magnetic phase diagrams consistent with the formation of a skyrmion pocket just below T_C .



(a) Crystal structure of the cubic series $\text{FePd}_{1-x}\text{Pt}_x\text{Mo}_3\text{N}$ (space-group $P4_32$). (b) Magnetic phase diagram of FePtMo_3N . (c) Helical wavelengths λ against x .

The magnitudes of ferromagnetic and DM exchanges are determined from the phase diagrams, demonstrating that the introduction of increasing amounts of Pt can be used to increase spin-orbit coupling in order to control the expected skyrmion lattice parameter between 140 nm and 65 nm while simultaneously increasing T_C .

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Thermally-robust magnetic skyrmion formation driven by crystal structure distortion in the lacunar spinels

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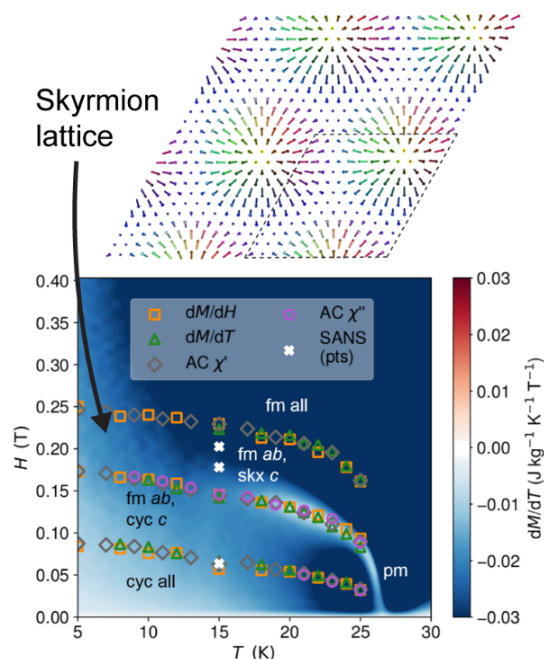
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The development of materials which stabilize magnetic skyrmions (magnetization spirals and vortices) and allow for control over their behavior is instrumental to the realization of skyrmion-based spintronic devices. The lacunar spinel family with the formula GaM_4Q_8 where $M=\text{V},\text{Mo}$; $Q=\text{S},\text{Se}$ is an attractive model system for identifying design criteria towards these goals as these highly correlated materials¹ are some of the first bulk systems discovered to host equilibrium chiral skyrmions with a large temperature stability range. We first report an experimental and computational characterization of GaMo_4Se_8 , revealing an intricate coupling between structural and magnetic phase behavior and equilibrium skyrmion formation over a wide temperature and field range. We prove the coexistence of two low-temperature phases with drastically different magnetic properties, switching between ferromagnetic and skyrmionic behavior. We then derive a general model for the behavior of the skyrmion-hosting phase which quantitatively reproduces all experimental reports in this space and demonstrates that skyrmion stability in the lacunar spinels and other systems with similar symmetry is largely controlled by the strength of magnetocrystalline anisotropy.² Our analysis identifies straightforward, general criteria for predicting skyrmion stability in a variety of materials and suggests a route for controlling the stability and properties of skyrmions *via* mechanical means.

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Experimentally and computationally derived magnetic phase diagram of GaMo_4Se_8 which includes a skyrmion region at all temperatures below T_c .

Mechanics and Adhesive Performance of Mussels on Roughness- and Geometry-controlled 3D printed Substrates

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Marine mussels have the remarkable ability to adhere to a variety of natural and artificial surfaces and maintain robust adhesive bonds under hostile environmental conditions. Although the molecular composition of mussel adhesives has been well studied, a mechanistic understanding of the physical origins of mussels' impressive adhesive strength remains elusive.³ Here, we investigated the role of substrate roughness and geometry in the adhesive performance of mussels. Using 3D printing, sandblasting, and laser texturing we created substrates with differing surface treatments and introduced these to mussels, which in turn adhered to the engineered surfaces via plaque-thread byssal structures. Tensile testing with *in situ* imaging was used to determine the adhesion strength and mechanical properties of the mussel adhesive plaques under various conditions. Our results inform the relationships between adhesive performance and substrate properties, give insight into the physical governing factors of mussel adhesion, and provide design criteria for development of synthetic adhesives for use on complex, textured surfaces.

This research was supported by the MRSEC Program of the National Science Foundation under Award No. DMR 1720256.

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A light meal: dietary acquisition and metabolism of bioluminescent compounds in the midshipman fishes

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Many organisms acquire, sequester, and use necessary biological molecules from their diet that they cannot produce themselves. Numerous bioluminescent organisms rely on dietary acquisition of substrates for bioluminescence, called luciferins. Luciferins are highly unstable molecules that are oxidized by enzymes called luciferases to produce light. Due to the instability of luciferins, bioluminescent organisms such as fireflies, the sea pansy, and ostracod crustaceans have evolved a luciferin storage mechanism to preserve the substrate until it is needed.^{1,2,3} We hypothesize that organisms that share luciferin via dietary acquisition have the same luciferin storage form. *Porichthys*, commonly known as midshipman fishes, produce their own luciferase but obtain luciferin from their diet of bioluminescent ostracods.⁴ A recent study on ostracods identified a more stable sulfated luciferin derivative that can be enzymatically converted into the active form of luciferin.³ Although previous work identified luciferin in its active form in various midshipman fish tissues and blood, the presence of luciferin derivatives has not yet been thoroughly investigated.⁵ Here, we use biochemical assays and liquid chromatography coupled with mass spectrometry to detect luciferin derivatives in midshipman fish tissues and eggs. Preliminary data indicate that, in midshipman fish eggs, a derivative of luciferin can be chemically converted into an active form of luciferin. Identifying luciferin derivatives in midshipman fish sets the stage for future studies on the convergent evolution of luciferin storage systems in these phylogenetically distant organisms.

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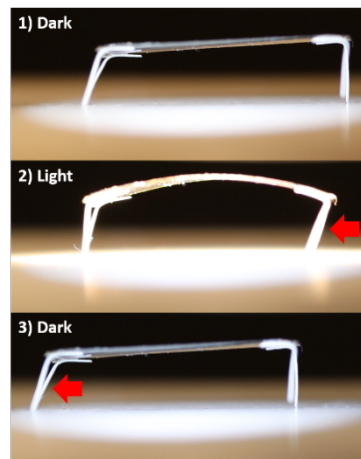
Programmable Photothermal Actuation using Novel Negative Photochromic Donor-Acceptor Stenhouse Adduct (DASA) Polymers

Jaejun Lee,^{a,b} Miranda Sroda,^a Younghoon Kwon,^b Sara El-Arid,^a Serena Seshadri,^a Luke Gockowski,^b Elliot Hawkes,^b Javier Read de Alaniz,^a and Megan T. Valentine^b

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Light-driven actuation has significant advantages including untethered operation, precise spatiotemporal activation, and the ability to operate in complex surroundings without significant modification. Here, we use a new class of molecular photoswitches, called donor-acceptor Stenhouse adducts (DASAs)¹⁻², to generate a novel but conceptually simple photo-responsive polymer bilayer actuator, capable of repeatedly lifting a load against the force of gravity and walking with an asymmetric leg design. We will present a synthesis pathway for chemically attaching DASA conjugates to poly(hexyl methacrylate) through norbornadiene click chemistry, and will demonstrate actuator performance. Importantly, we can leverage the different time scales of photothermal and photochemical responses of DASAs to achieve dynamic material control, including the ability to switch on and off actuation. Our results highlight the promising benefits of high molar absorptivity, negative photochromism, and visible light absorption of DASAs for actuation.



Crawling DASA robot powered by light. Red arrows indicate moving direction at each stage.

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Asymmetric Miktoarm Star Polymers via ROMP

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Asymmetric miktoarm star polymers are potentially useful in applications ranging from thermoplastic elastomers to drug delivery.¹ Despite such promise, synthetic complexity remains a major bottleneck to their widespread utilization. Here, we introduce a new synthetic strategy that simplifies the synthesis of asymmetric miktoarm star polymers using grafting-through polymerization of a norbornene-functionalized “macromonomer” to construct the junction,² followed by efficient termination to install a single disparate type of arm.³ Experiments and theory indicate the self-assembly of these materials is controlled by the average number of macromonomer-derived arms, which is easily controlled through reaction stoichiometry. Due to the functional group tolerance of Grubbs catalysis, a wide variety of AB_n and $A(BA')_n$ miktoarm star polymers can be produced from different A and B block chemistries.

This research is based upon work supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Award Number DE-SC0019001 and the Mellichamp Academic Initiative in Sustainability. The research reported here made use of shared facilities of the National Science Foundation (NSF) materials research Science and Engineering Center at UC Santa Barbara, DMR-1720256. The UCSB MRSEC is a member of the Materials Research Facilities Network (www.mrfn.org).

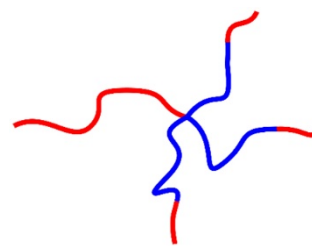


Illustration of an asymmetric miktoarm star polymer.

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Solid-Liquid Transition of Deformable and Overlapping Active Particles

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Experiments and theory have shown that cell monolayers and epithelial tissues exhibit solid-liquid^{1,2} and glass-liquid transitions³. These transitions are biologically relevant to our understanding of embryonic development, wound healing, and cancer. Current models typically consider purely two-dimensional monolayers with no overlaps between neighboring cells^{4,5}. In reality, overlaps are important, and they may be precursors of cell extrusion -- a key biophysical process to maintain homeostasis in epithelial tissues. Here, we use a multi-phase field model to study the solid-liquid transition in a confluent monolayer of deformable cells, which can overlap. When cells overlap rather than deform, we find that the melting transition changes from continuous to discontinuous, and that there is an intermittent regime close to the transition, where solid and liquid states alternate over time. By studying the dynamics of 5- and 7-fold disclinations in the hexagonal lattice formed by the cell centers, we observe that these correlate with spatial fluctuations in the cellular overlap, and that cell extrusion tends to initiate near 5-fold disclinations.

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Engineering interfacial strain gradients in biphasic MnCoSb–(Ti,Zr)CoSb half Heusler composites

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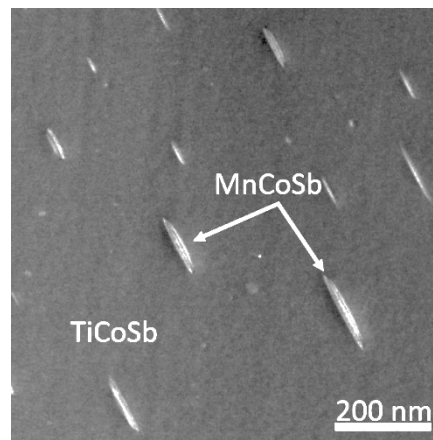
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An antisymmetric exchange interaction known as the Dzyaloshinskii-Moriya (DM) interaction gives rise to skyrmions and novel magnetic textures in non-centrosymmetric materials. Recent first principle calculations suggest the DM interaction can be realized in centrosymmetric crystals by breaking symmetry through the application of a strain gradient.¹ The Heusler system MnCoSb–(Ti,Zr)CoSb is a prime candidate for exploring this phenomenon as it phase separates into a nonmagnetic and highly tunable Ti_{1-x}Zr_xCoSb phase and a centrosymmetric magnetic MnCoSb phase with semi-coherent interfaces similar to previously studied half Heusler/Heusler composites.^{2,3} Precise control over microstructure and therefore interfacial strain is obtained through chemistry and processing. We explore the phase separation characteristics of this system using electron microscopy and X-ray diffraction, which are supported by density functional theory calculations. Future work will include relating magnetic properties of the strained precipitates to systematically controlled changes in microstructure.

This work is supported by the Materials Research Science and Engineering Center at UCSB: MRSEC NSF DMR 1720256 through IRG-1 and made use of the central facilities of the Materials Research Laboratory.

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HAADF-STEM image showing MnCoSb embedded in TiCoSb matrix.

Bioelectronic composites using conjugated polyelectrolytes

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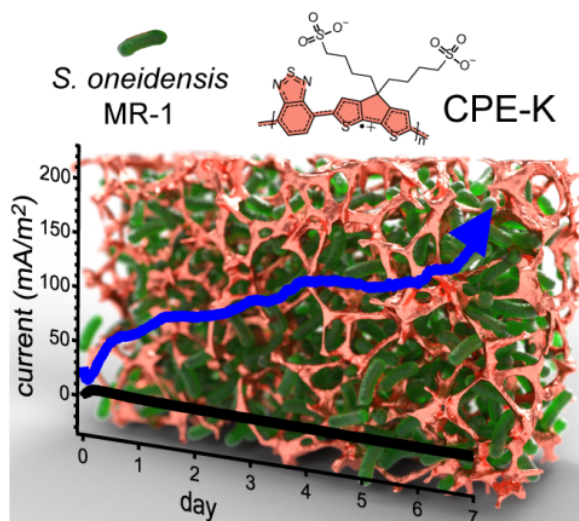
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Composites, in which two or more material elements are combined to provide properties unattainable by single components, have a historical record dating to ancient times. Few have included a living microbial community as a key design element. A logical basis for enabling bioelectronic composites stems from the phenomenon that certain microorganisms transfer electrons to an external surface, such as an electrode. Indeed, a series of bioelectrochemical systems based on microbial electroactivity has been developed.¹ Integration of materials at the microbe/electrode interface has improved electron transfer efficiency and cell adhesion, but charge injection/extraction is still largely restricted to the immediate proximity between bacteria and the external electrode.^{2,3} We show that the conjugated polyelectrolyte CPE-K functions as a conductive matrix to electronically connect a three-dimensional network of *Shewanella oneidensis* MR-1 to an external gold electrode, thereby increasing biocurrent by ~150-fold over standard control biofilms. The biocomposites spontaneously assemble from solution into an intricate arrangement of cells within a conductive polymer matrix. This approach can impact bioelectrochemical technologies that benefit from addressing cells beyond the confines of the electrode surface. The impact of CPE-K concentration on bioelectronic composite performance will be discussed, along with an evaluation of electroactive surface area and charge transfer resistance.



A conductive polymer matrix couples electroactive microbes with electronic contacts.

Funding was provided by the Institute for Collaborative Biotechnologies (ICB) under grant W911F-09-D-0001 from the U.S. Army Research Office. S. R. M is grateful for funding from the National Science Foundation Graduate Research Fellowships Program (NSF GRFP).

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First-principles study of Ga₂O₃: exploring higher thermal conductivity and growth mechanisms

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Monoclinic gallium oxide (Ga₂O₃) has promising applications in high-power and high-frequency electronics due to its wide bandgap. However, practical device applications are hampered by the low thermal conductivity of Ga₂O₃. To improve the thermal properties of Ga₂O₃ devices, we propose to alloy Ga₂O₃ with Al₂O₃, forming a low-energy ordered structure at the 50% concentration.¹ We investigate the lattice thermal conductivity of monoclinic Ga₂O₃ and of the ordered AlGaO₃ alloy using density functional theory.² We find that the thermal conductivity of AlGaO₃ is raised by more than 70% compared to Ga₂O₃. The enhancement is ascribed to (a) increased group velocities and (b) reduced anharmonic scattering rates due to the reduced weighted phase space. In addition, the growth rate and crystal quality of Ga₂O₃ thin films are limited by suboxide desorption. It has been reported that the growth rate of Ga₂O₃ in molecular beam epitaxy can be enhanced by the additional indium (In) flux.³ We employ density functional theory to explore the adsorption of Ga and In adatoms on the (010) surface and to investigate the desorption energy of the suboxide in the presence of adatoms.⁴ We find that co-adsorption of two In and two Ga adatoms is energetically favorable, and the corresponding desorption energy of the suboxide is raised. Therefore, the desorption rate is reduced by the co-adsorption of Ga and In adatoms. The findings offer an avenue towards improved heat dissipation from Ga₂O₃ devices and elucidate the growth mechanism of Ga₂O₃ thin films.

The work was supported by the GAME MURI of the Air Force Office of Scientific Research.

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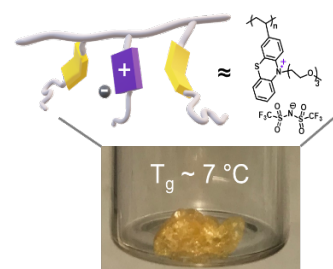
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Soft and Electrically-Active Redox-Active Polymeric Ionic Liquids

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Polymeric ionic liquids (PILs) are promising candidates for soft electronics owing to their capability to conduct ions. They are amorphous polymers with ionic functionalities on the side chain with a counterion that can lead to a low glass transition temperature (T_g). However, the relatively high T_g of many redox-active polymers make it challenging to fabricate soft electronics. To overcome this issue, there have been efforts to decrease the T_g of redox-active polymers by increasing the length of the aliphatic chains in between tethered charge-conducting side chains and the backbone. However, this structural change can negatively affect charge transport properties by spatially separating the redox active groups. Here, we present a modular synthetic platform that places the redox-active PIL bearing a phenothiazine-bis(trifluoromethanesulfonyl)-imide (TFSI) ionic liquid side chains close to the backbone and incorporates a short ethylene glycol unit on the phenothiazine to lower the T_g . Enhanced charge transport was successfully demonstrated upon oxidation and with increasing amounts of the TFSI anion while maintaining the PIL properties. In this presentation, we will demonstrate that both electrical and mechanical properties could be enhanced with our novel polymeric design for future applications.



Soft and electrically-active PIL with low T_g . Efficient charge transport attained by the closely located redox-active units.

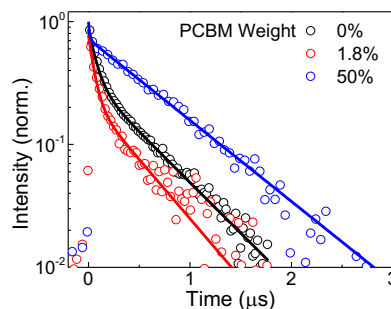
Simultaneous Characterization of Thermal Transport and Photocarrier Dynamics in Organic Semiconductors

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In this paper, we retrieved both the carrier dynamics and thermal transport features simultaneously for polymer: fullerene blends by utilizing laser-induced transient grating spectroscopy (TGS) within the time window of microseconds over micron distances. By applying an appropriate model containing the two processes, it was resolved that the carrier dynamics are determined by a combined trapping and recombination process, while heat is propagated through diffusion. Specifically, the crystalline structure of P3HT was barely changed at low PCBM loading, resulting in similar first-order carrier dynamics. However, when PCBM loading was above the miscibility limit, the increased donor-acceptor interfaces ensured efficient dissociation of excitons into free carriers such that bimolecular recombination emerges. The first-order decay rates were located in the range of $10^7 \sim 10^8 \text{ s}^{-1}$, and the second rates were at the order of $10^{-9} \sim 10^{-8} \text{ cm}^3/\text{s}$, which were in good agreement with other experimental reports. In addition, thermal diffusivity decreased from $0.44 \text{ mm}^2/\text{s}$ to $0.21 \text{ mm}^2/\text{s}$ upon increasing PCBM content, indicating that thermal diffusion was weakened due to phonon scattering at domain boundaries. Such features are beneficial for improving heat dissipation or thermoelectricity by simply engineering the polymer: fullerene blend ratio. This characterization method was also proved applicable for PCDTBT, making it a reliable tool studying physical properties in organic semiconductors.



The decaying of the transient grating intensity in time for different PCBM concentration.

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Mussel inspired polymers for flexible electronics applications

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Electroless plating of solid metals from a solution onto a catalytically active surface has been widely used in the printed circuit board industry for production of wiring layers and inter-layer (via) connections. Smooth substrate surfaces, like polyimide (PI) for flexible electronics applications, are particularly challenging as the electrolessly plated metal tends not to adhere to the surface. It is therefore desirable to develop new chemistries that can be used for adhesion promotion between the polyimide substrate and the deposited copper. Herein, we introduce a mussel-inspired universal adhesive moiety, dopamine, as a side group to a water soluble polymer backbone and demonstrate its application as an adhesion promotion layer for electroless plating of flexible substrates. When the polymer is deposited on a substrate surface, the DOPA moiety reacts with the substrate and adheres to it while the polymer chain extends and folds to generate a smoother outer surface through minimizing the surface energy, creating a smooth and uniform coat of deposited copper.

Weyl semimetal thin film $\text{Eu}_{1-x}\text{Sm}_x\text{TiO}_3$ on LSAT (001): field-polarized long-range order and interfacial ferromagnetism

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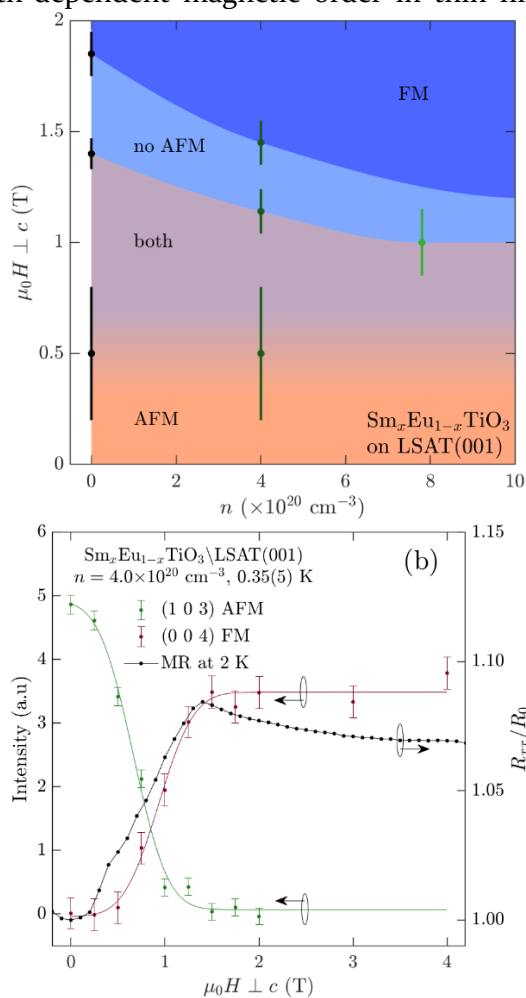
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We report on the evolution of the average and depth-dependent magnetic order in thin film samples of biaxially strained and electron-doped EuTiO_3 for samples across a doping range <0.1 to $7.8 \times 10^{20} \text{ cm}^{-3}$. Under applied in-plane field, the G-type antiferromagnetic ground state undergoes a continuous phase transition to in-plane field-polarized ferromagnetism. The critical field for ferromagnetism decreases with itinerant carriers, yet the field evolution is qualitatively similar across the doping range. Unexpectedly, we observe interfacial ferromagnetism with saturated Eu moments at low fields preceding ferromagnetic saturation throughout the bulk of the semimetallic film. We discuss the implications of these findings for the unusual magnetotransport, particularly the anisotropic magnetoresistance and the purported topological Hall effect. These results may hold significance for other magnetic Weyl semimetal systems.

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(a) Field-Carrier concentration phase diagram based on the neutron diffraction. (b) Neutron diffraction order parameters of the semimetallic sample for antiferromagnetic (green) and ferromagnetic (red) reflections. Overlaid in black is magnetoresistance.

The effect of the counter ion structure on the spatial distribution and molecular configuration of charge carriers in solid state electrochemically doped conjugated polymers

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In a chemically doped or electrochemically doped conjugated polymer, electronic charge carriers are inherently associated with a countercharge in the form of an atomic or molecular counterion. It is expected that the structure of the counter ion will affect its distribution in the polymer film along with that of associated electronic charge carriers. Furthermore, the effect of counter ion structure on the charge storage configuration (i.e. polaron vs. bipolaron) is unknown. Here, we quantify the polaron to bipolaron ratio and the distribution of charge carriers between aggregated and amorphous domains as a function of the counter ion structure in semicrystalline conjugated polymer films. We employ an organic electrochemical transistor with a cation tethered polymeric ionic liquid (PIL) as the gate dielectric, where the size and structure of the mobile anionic counterion in the PIL can be varied to modulate the counterion that is associated to charge carriers in the semiconductor. Operando electron paramagnetic resonance and in-situ device measurements reveal the spin concentration as a function of the gate bias for a range of counter ions. This is paired with in-situ optical spectroscopy to determine the distribution of charge carriers between amorphous and aggregated domains.

Super-soft solvent-free bottlebrush elastomers for touch sensing

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Pressure sensors with high sensitivity have uses ranging from pulse monitoring and plantar pressure measurement (10–100 kPa) to *in vivo* intraocular and intracranial pressure measurement (1–10 kPa). The sensitivity of capacitive pressure sensors is primarily determined by the modulus of a dielectric layer that reversibly deforms to produce an electrical signal. Crosslinked polymers provide a means to achieve good dielectric properties with low modulus relative to inorganic materials. Unfortunately, the mechanical properties of conventional linear polymer networks are constrained such that a lower limit on softness translates to poor capacitive pressure sensor performance. Here, we overcome this limitation by leveraging the intrinsic “super-soft” characteristic of bottlebrush polymers, which can be crosslinked to form solvent-free networks with moduli in a range matching that of biological tissues (1–100 kPa). A simple light-induced crosslinking strategy is introduced to facilitate device fabrication. Parallel plate capacitive pressure sensors constructed with these bottlebrush polymer networks exhibit up to a 53× increase in sensitivity compared to commonly used elastomers, e.g., PDMS (Sylgard 184). The sensors show pressure resolution on the order of 0.1 kPa, capable of differentiating subtle forces in the light touch regime. Transparent and flexible sensors fabricated using indium-tin-oxide (ITO)-coated poly(ethylene terephthalate) (PET) electrodes are shown to be functional in a bent configuration. This combination of contemporary synthetic chemistry and application-driven materials design accentuates the opportunities available at the intersection of science and engineering to advance soft, flexible, and biocompatible devices.

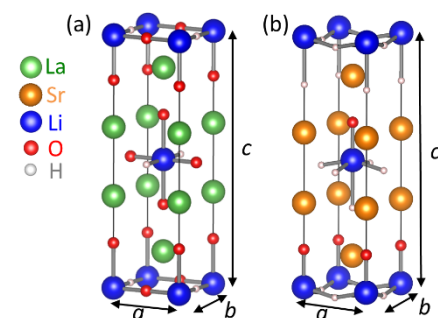
Defect chemistry and hydrogen transport in La/Sr-based oxyhydrides

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Oxyhydrides are crystalline materials in which the anionic sites exhibit mixed occupation by hydrogen and oxygen. Several oxyhydrides have demonstrated high hydride ionic conductivity and are being actively explored as solid-state hydrogen electrolytes for use in fuel cells [1]. The relevant properties of these materials, stability and ionic conductivity, are intrinsically tied to their defect chemistry, which is not yet understood. We perform first-principles calculations of native point defects in the oxyhydrides La_2LiHO_3 and $\text{Sr}_2\text{LiH}_3\text{O}$ to determine which defects are most prevalent and most determinative of the crystals' properties. We find that hydrogen vacancies (V_{H}^+) are most critical for hydride conduction, and they can be readily incorporated under H-poor, O-rich conditions. Disorder in the form of other defects, including hydrogen interstitials (H_i^+) and anionic antisites (O_{H}^- and H_{O}^+) will occur and, particularly in the case of the more conductive $\text{Sr}_2\text{LiH}_3\text{O}$, improve the chemical stability. We propose optimal synthesis conditions for these materials to optimize their stability and conductivity for applications in solid-state hydrogen fuel cells.



Crystal structures of the oxyhydrides
(a) La_2LiHO_3 and (b) $\text{Sr}_2\text{LiH}_3\text{O}$.

Computational resources were provided by NERSC and by the Center for Scientific Computing (CSC) at UCSB. Supported for this research was provided by the National Science Foundation (Graduate Research Fellowship Program, Grant No. 1650114) and by the US DOE Office of Science (Grant No. DE-FG02-07ER46434).

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Effect of Sintering Temperature on the Crystal Structure, Phase Stabilization, and Electrical Properties of $\text{BaFe}_{0.7}\text{Ta}_{0.3}\text{O}_{3-\delta}$ Ceramics

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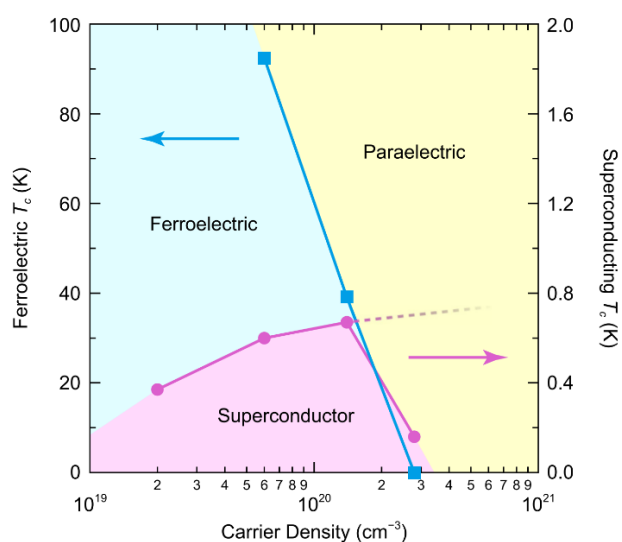
Temperature independent chemical sensors are needed for optimization of emission control in fossil-fuel based power plants and automotive engines operating at extreme temperatures. Unfortunately, traditional metal oxide based oxygen sensors tend to fail under extreme operating conditions (500-800 °C). In course of finding novel functional materials, perovskite oxides have drawn considerable interest due to their thermal stability in extreme conditions. In this context, the present work was performed on the processing, characterization and performance evaluation of $\text{BaFe}_{0.7}\text{Ta}_{0.3}\text{O}_{3-\delta}$ (BFTO₃₀) ceramics for oxygen sensor applications. BFTO compounds were synthesized using conventional solid-state reaction route. The effect of sintering temperature (1200-1350 °C) was significant on the crystal structure and phase of BFTO ceramics. X-ray diffraction patterns of sintered BFTO reveals that there is a structural transformation with increasing temperature. Electron microscopy analyses of the surface morphology indicate the BFTO samples sintered at 1350°C exhibit dense, grain structure while those sintered at lower temperature exhibit porous morphology. The corresponding dielectric properties studies indicate that the dielectric constant and its frequency dispersion depend on the phase and microstructure of the BFTO ceramics. Oxygen sensor testing, which is currently progressing, results of these BFTO ceramics are encouraging.

Ferroelectric enhancement of superconductivity in compressively strained SrTiO₃ films

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SrTiO₃ is an incipient ferroelectric on the verge of a polar instability, which is avoided at low temperatures by quantum fluctuations. Within this unusual quantum paraelectric phase, superconductivity persists despite extremely dilute carrier densities. Ferroelectric fluctuations have been suspected to play a role in the origin of superconductivity by contributing to electron pairing. To investigate this possibility, we used optical second harmonic generation to measure the doping and temperature dependence of the ferroelectric order parameter in compressively strained SrTiO₃ thin films. At low temperatures, we uncover a spontaneous out-of-plane ferroelectric polarization with an onset that correlates perfectly with normal-state electrical resistivity anomalies. These anomalies have previously been associated with an enhancement of the superconducting critical temperature in doped SrTiO₃ films, directly linking the ferroelectric and superconducting phases. We develop a long-range mean-field Ising model of the ferroelectric phase transition to interpret the data and extract the relevant energy scales in the system. Our results support a long-suspected connection between ferroelectricity and superconductivity in SrTiO₃, but call into question the role played by ferroelectric fluctuations.



Doping-temperature phase diagram of compressively strained SrTiO₃

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Dynamic bottlebrush networks: self-healing in super soft materials

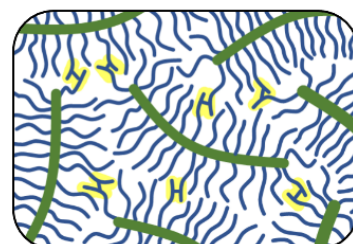
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Bottlebrush polymer networks have very desirable properties due to their unusual architecture, resulting in materials that are unusually soft and elastic.¹ These mechanical properties make this an attractive material for various advanced applications, including biomimetic materials. Herein, we report a bottlebrush polymer network composed of polyester sidechains which, in the presence of a strong Lewis Acid, undergo exchange reactions to allow for network rearrangement. Though fully crosslinked, these materials can completely relax stress in as little as 20 minutes at elevated temperatures due to the dynamic crosslinks, thereby behaving as a covalently adaptable network.² The stress relaxation behavior exhibits a strong Arrhenius dependence with activation energies of $89 \pm 2 \text{ kJ mol}^{-1}$ regardless of crosslinker loading. Through tuning of either the crosslinker loading or the length of the bottlebrush polymer backbone, this system spans modulus values from 10^4 to 10^6 Pa, well below the accessible modulus of linear polymer analogs. These networks also demonstrate extensibility, reaching strains as high as 350% before failure. Finally, the ability to heal is demonstrated with recycling studies which show greater than 85% recovery of toughness compared to pristine samples. The ability to repair these materials represents a major advance for bottlebrush polymer networks, whose unique mechanical properties are highly desirable for various applications.



Bottlebrush polymer networks are polymers composed of a rigid backbone (in green) with flexible sidechains (in blue) extending outward. Here, the dynamic crosslinks are highlighted (in yellow).

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Self-regulating photochemical Rayleigh-Bénard convection using a highly-absorbing organic photoswitch

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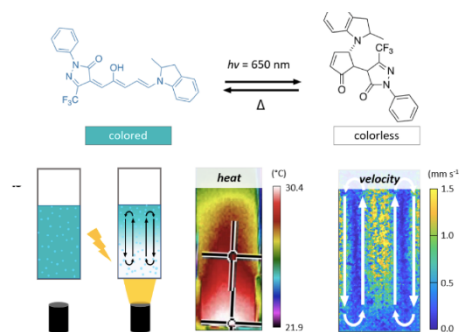
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Autonomous control of liquid motion is vital to the development of new actuators and pumps in fluid systems. Recently, light has been recognized as a formidable tool for non-invasive, wavelength-selective, remote control over liquid motion with high spatial and temporal resolution. In this work, we identify unique features of a donor acceptor Stenhouse adduct (DASA), a highly-absorbing negatively photochromic molecular switch, that enable its use for the control of fluid velocity. The balance between convective mass transport and the tunable rate of the back reaction of DASA offers a unique handle by which we can control the self-regulatory properties of the system. For solvents in which DASA 3.0 has a fast back reaction, the dynamic steady state achieved in solution produces a self-regulating thermal gradient that can drive fluid flow at a constant velocity. In solvents in which DASA bleaches rapidly and has a slow back reaction, it operates as an effective “off-switch” after the solution has entirely bleached and the thermal gradient dissipates. Leveraging features of DASA’s chemical properties and solvent-dependent reaction kinetics, we demonstrate its use for photo-controlled Rayleigh-Bénard convection to generate dynamic, self-regulating flows with unparalleled fluid velocities ($\sim\text{mm s}^{-1}$) simply by illuminating the fluid with visible light. The exceptional absorbance of DASAs in solution, uniquely controllable reaction kinetics and resulting spatially-confined photothermal flows present exciting opportunities for optofluidics applications requiring tunable flow behavior.

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The photothermal effect and solvent dependent switching kinetics of a molecular photoswitch (DASA) is leveraged to enact self-regulatory control over convective fluid motion

Magnetostructural instabilities in topological semimetals

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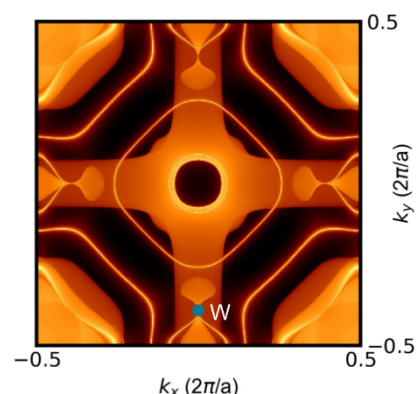
We present first-principles calculations suggesting that the ferromagnetic phase of cubic antiperovskite Mn_3ZnC is a nodal line Weyl semimetal. Electronic structure features that are the hallmark of this nodal line state—a large density of linear band crossing near the Fermi level—can also be interpreted as signatures of structural and magnetic instability. In fact, it is known that Mn_3ZnC transitions upon cooling from a paramagnetic to a cubic ferromagnetic state under ambient conditions and then further into a non-collinear tetragonal phase at a temperature between 250 K and 200 K. The existence of Weyl nodes and their destruction via structural and antiferromagnetic ordering is likely relevant to a range of magnetostructurally coupled materials.

Preliminary experimental results on additional antiferromagnetically-ordering semimetal systems will also be presented.

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A constant-energy cut of simulated Weyl nodes and surface states in the ferromagnetic phase of Mn_3ZnC

Boron dangling bonds in hexagonal boron nitride for quantum information science

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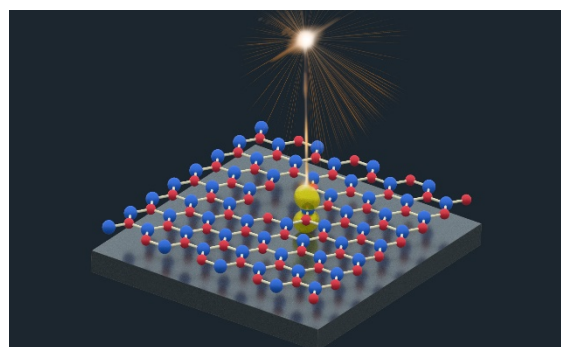
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Hexagonal boron nitride (h-BN) is a two-dimensional, layered material with excellent stability and ultra-wide band gap; these properties make h-BN an appealing host for so-called quantum defects, which are an ideal platform to realize applications in quantum information science. Extensive experimental efforts have uncovered a plethora of single-photon emitters in h-BN that may be utilized as quantum defects, but the microscopic origin of these emitters proved elusive. Using first-principles density functional theory, we have studied the defect chemistry of h-BN [1] and identified boron dangling bonds as the likely source of the observed single-photon emission near 2 eV [2]. Boron dangling bonds give rise to a linearly polarized optical transition at 2.06 eV with minimal coupling to phonons, consistent with experimental reports. The system possesses a singlet ground state, with a metastable triplet state that could be used to realize spin-qubit and metrology applications. Our results provide a coherent narrative to the story of single-photon emission in h-BN and offer exciting prospects for engineering efforts, now that the microscopic origin of the emission has been identified.



An artist's rendition of the boron dangling bond emitting a single photon.

The research reported here was primarily supported by the NSF through the MRSEC at UC Santa Barbara, DMR-1720256 (Seed) and by DOE-BES.

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$\text{Li}_5\text{VF}_4(\text{SO}_4)_2$, a high voltage fluorosulfate lithium-ion cathode material

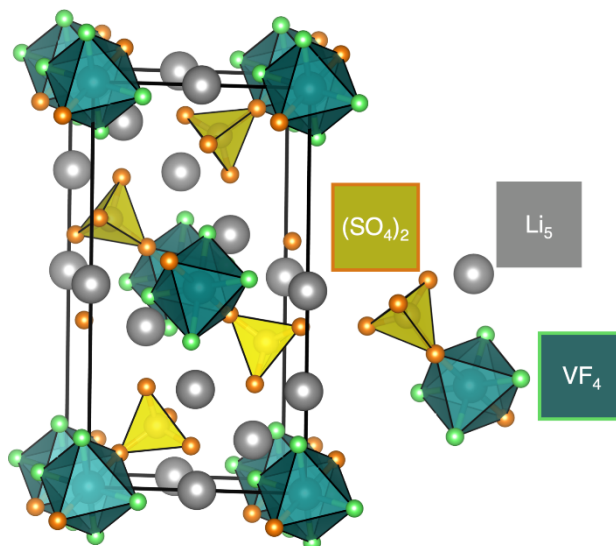
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Lithium ion batteries play a critical role in modern society, allowing us to use lightweight and powerful portable electronics. As a greater percentage of vehicles in the world become electric, the need for higher energy density batteries becomes more pressing.

A new compound, with a previously unknown structure $\text{Li}_5\text{VF}_4(\text{SO}_4)_2$ has been developed as a potential high voltage cathode material for lithium ion batteries, and increasing operating voltage is one way to increase the energy density of the cathode material. Incorporation of fluorine increases operating voltage due to its high electronegativity, and the sulfate polyanion increases voltage due to the inductive effect.¹ We present the first synthesis of $\text{Li}_5\text{VF}_4(\text{SO}_4)_2$, which is achieved using solvothermal methods, crystal structure solution, and initial electrochemical characterization. Some lithium can be extracted from the material at high voltage, however it is difficult to quantify above the stability window of conventional organic electrolytes (about 4.3 V). Going beyond this high potential will require alternate electrolytes that are stable at higher potentials.



Crystal structure of $\text{Li}_5\text{VF}_4(\text{SO}_4)_2$

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Hybrid Ruthenium Halide Perovskites and Related Phases

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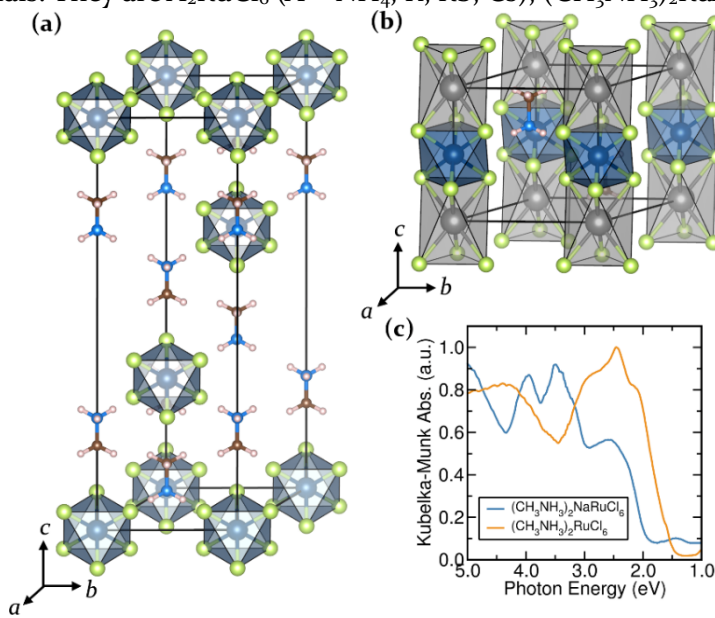
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Hybrid halide perovskites have expanded rapidly since the discovery of excellent optoelectronic properties of $APbX_3$ perovskites (where A is monovalent organic cation such as $CH_3NH_3^+$ and X is halide such as Cl^- , Br^- or I^-). However, the toxic nature of lead perovskites challenges their large-scale application and replacement of lead with nontoxic metals could lead to environmentally-friendly perovskites. Significant progress has been made on various ABX_3 , A_2BX_6 , $A_2B'B''X_6$ and other types of lead-free perovskites by tuning the A , B and X sites. However very little is known about hybrid halide perovskites of transition metals. In this work, we describe a series of hybrid perovskite Ru halides and related materials. They are A_2RuCl_6 ($A = NH_4, K, Rb, Cs$), $(CH_3NH_3)_2RuX_6$ ($X = Cl$ or Br) and $(CH_3NH_3)_2MRuX_6$ ($M = Na, K$ or Ag ; $X = Cl$ or Br). A_2RuCl_6 phases show K_2PtCl_6 -type vacancy ordered cubic structures while the $(CH_3NH_3)_2RuX_6$ phases are rhombohedrally distorted version of these structures. The $(CH_3NH_3)_2MRuX_6$ phases contain 1D chains of alternating face-sharing RuX_6 and MX_6 polyhedra surrounded by methylammonium cations (MA). The MA cations form weak $N-H\cdots X$ hydrogen bonds to stabilize $(CH_3NH_3)_2RuX_6$ and $(CH_3NH_3)_2MRuX_6$. We have studied the optical and magnetic properties of these compounds. The approach presented opens up new avenues for lead-free perovskites.

This work is supported by the

U. S. Department of Energy, Office of Science, Basic Energy Sciences, under the SC0012541 Grant. The authors acknowledge Materials Research Science and Engineering Center (MRSEC) (Grant No. NSF DMR 1720256) for providing access to its shared facilities created at UC Santa Barbara. PV thanks the Department of Science & Technology (DST), Govt. of India for an Overseas Post-doctoral Visiting Fellowship (Fellowship Award No. JNC/AO/A.0610-1(3)/2018-03), managed by Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India.

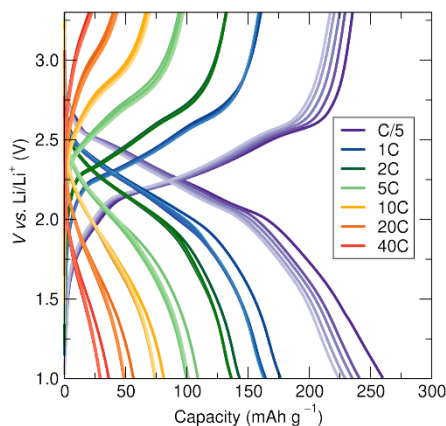


Crystal structures (unit cells) of (a) $(CH_3NH_3)_2RuCl_6$ (b) $(CH_3NH_3)_2NaRuCl_6$. (c) UV/Vis/NIR absorption spectra of $(CH_3NH_3)_2RuCl_6$ and $(CH_3NH_3)_2NaRuCl_6$.

(W_{0.2}V_{0.8})₃O₇ as fast-cycling electrode in lithium ion batteries**K. Wyckoff,^a J. Bienz,^b and R. Seshadri^{a,b}**^aDepartment of Materials Science and Engineering^bDepartment of Chemistry

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As batteries have become ubiquitous in a range of applications, there is a growing need to improve the cyclability, cycling rates, capacity, and lifetime of the devices through both choice of material, and the morphology and architecture. Our studies are aimed at materials that are intrinsically conductive and capable of faster cycling performance. Transition metal oxides derived from the shearing of perovskite-like octahedral slabs, in order to introduce edge-connected moieties, leads to so-called shear phases that promise effective ion and charge transport and therefore fast charging.¹ These design rules have led to discovery of a number of transition metal oxides, such as (W_{0.2}V_{0.8})₃O₇, that have shown notable capacity retention at high cycling rates in micron sized particles.² Extensive data investigating the fundamental surface and bulk properties and cycling performance of this compound have been collected.



Galvanostatic charge and discharge curves for bulk (W_{0.2}V_{0.8})₃O₇ from C/5 up to 40C.

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Insensitivity of Sterically-Defined Helical Chain Conformation to Solvent Quality in Dilute Solution

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Helices are a common secondary structure in both synthetic and biopolymers. Helical polymers can be either relatively stiff (rod-like), or have highly dynamic helical secondary structures. In this work, we study the helical secondary structure formed in polypeptoids–poly(*N*-substituted glycines). Unlike the helical structures in biological macromolecules that are usually induced by hydrogen-bonding, these polypeptoid helices are primarily driven by steric interactions from homochiral, bulky side chains. By comparing the chain conformation of helical polypeptoids (with homochiral side chains) and its coil counterpart (with racemic side chains) in dilute solution, we study the interplay between polymer–polymer, polymer–solvent interactions and interactions that impose the secondary structure. Small angle neutron scattering (SANS) of the polypeptoids reveals that the helical polypeptoids are locally stiffer but overall flexible in all solvents examined. The chain conformation (in terms of radius of gyration, R_g) of both helical and coil polypeptoids appears to be relatively constant as solvent quality (parameterized by the second virial coefficient, A_2) increases. Potential effects from the bulky, chiral side chains dominating chain conformation are excluded by comparing to another coil polypeptoid devoid of side chain chirality, which showed a similar trend in R_g as a function of A_2 . The results indicate that chain conformation of the sterically-defined helical polypeptoid in dilute solution is relatively insensitive to solvent quality, nor is it dominated by the chirality of the side chains. It is likely that the specific interactions between polypeptoid segments dominate the chain shape in this type of polypeptoids as opposed to polymer–solvent interactions and energetic contributions from the helical secondary structure.

The research reported here is supported by the National Science Foundation (NSF) Division of Materials Research Polymers program (DMR-1608297).

Giant Kohn Anomaly in Dirac Semimetals

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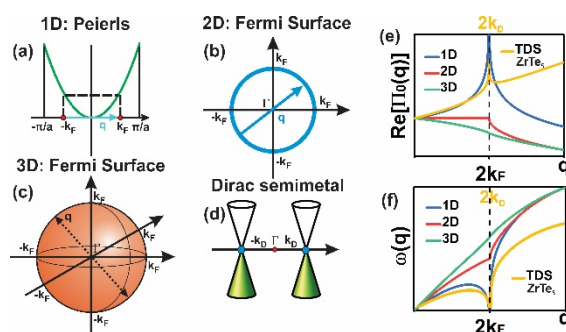
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Topological Dirac semimetal (TDS), as a new class of topological electronic state, possesses 3D Dirac fermions protected by topology and symmetry. Many unique electronic properties have been well studied; however, few phonon behaviors of TDS have been discussed. In this work, via ab initio simulation and field-theoretical derivation, we report the existence of strong Kohn anomalies in Dirac semimetals Cd_3As_2 , ZrTe_5 and Na_3Bi which originate from the electron-phonon interaction (EPI) associated with the Dirac nodes. Because the Fermi surface of TDS has distinct nesting condition with 3D Dirac nodes, Kohn anomaly effect in TDS only resorts specific selection rules: inter- and intra-nodes. All of the TDSs show extremely low thermal conductivities at room temperature. Our work proposes a novel potential mechanism of phonon softening to drive low thermal conductivity in topological materials.³

This work is based on research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering through the Early Career Research Program under the award number DE-SC0019244.

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Schematic representations of the Kohn anomaly associated with different Fermi-surface nesting.