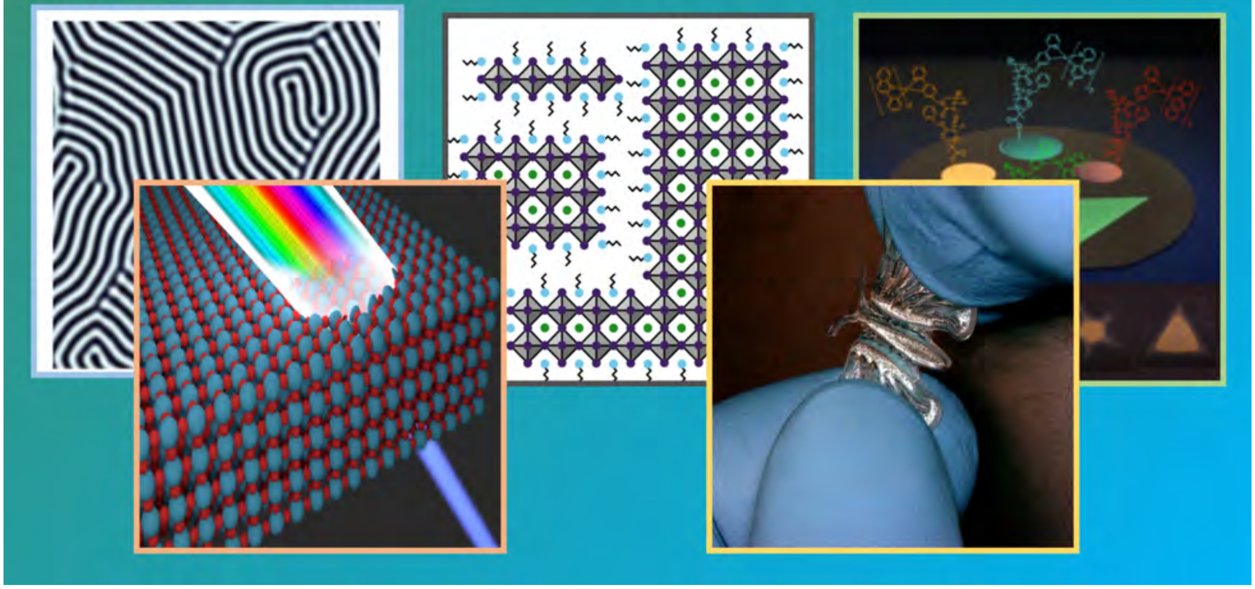
Materials Research Laboratory: An NSF MRSEC

Materials Research Outreach Program, 2018

Wednesday January 31st and Thursday February 1st 2018

Corwin Pavilion, UC Santa Barbara

Schedule, Biosketches, and Poster Abstracts



Materials Research Outreach Program

January 31st and February 1st, 2018 at the Corwin Pavillion

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Support for this symposium is generously provided by the Materials Research Science and Engineering Center Program of the National Science Foundation and the University of California, Santa Barbara

NSF DMR 1720256

MRSEC

UNIVERSITY OF CALIFORNIA SANTA BARBARA

About the MROP

Initiated in 1999 under the leadership of Professor Ed 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 local start-ups –– the MROP has emerged as the principal occasion to hear about and share UCSB research in the broad Materials arena.

The MROP has traditionally encouraged many new faculty members from a cross-section of UCSB Departments to showcase their research vision, leading to the nucleation of numerous collaborations. Key academic scientists, 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 2018 MROP, and thank you for your continued support. We hope you enjoy the MROP as much as we enjoy organizing it.

Session 1, Wednesday Morning, January 31, 2018, Corwin Pavilion

8:15 am	*Breakfast*	
8:45 am	*Opening remarks by* **Dean Alferness**, **Dean Wiltzius**, *and* **VC Incandela**	
9:00 am	**Douglas Fabini** *UCSB, Materials*	Main-Group Halide Perovskites: Structural And Dynamical Insights for Photovoltaic Performance
9:30 am	**Kerstin Schierle-Arndt** *BASF*	CARA - California Research Alliance by BASF
10:00 am	*Refreshment Break*	
10:30 am	**Siddharth Dey** *UCSB*, Chemical Engineering	Studying Heterogeneity in Biological Systems
11:00 am	**Morgan Schulze** *UCSB*, Chemical Engineering	Bridging Synthesis and Self-Assembly in Advanced Soft Materials
11:30 am	**Gab Menard** *UCSB, Chemistry & Biochemistry*	Abundant Metal Complexes for Chemical or Electrochemical Energy Storage
12:00 pm	*Lunch*	

Session 2, Wednesday Afternoon, January 31, 2018, Corwin Pavilion

1:30 pm	**Kristin Ceder-Persson** *UC Berkeley and LBNL*	The Materials Project for Accelerated Materials Design and Discovery
2:00 pm	**Zvonimir Dogic** *UCSB, Physics*	Autonomous Motility in Soft Active Matter
2:30 pm	*Refreshment Break*	
3:00 pm	**James Rogers** *Apeel Sciences*	Beyond "Chemicals" - Microstructure in Agriculture
3:30 pm	**CHEETHAM LECTURE** **Stuart Rowan** *University of Chicago*	Design and Synthesis of Adaptive Polymeric Materials
4:30 pm	*Posters and Reception*	

Session 3, Thursday Morning, February 1, 2018, Corwin Pavilion

8:30 am	*Breakfast*	
9:00 am	**Dan Gianola** **Stephen Wilson** *UCSB, Materials*	IRG-1: Magnetic Intermetallic Mesostructures
9:30 pm	**Alexandra Bayles** *UCSB, Chemical Engineering*	Liquids as Solids: Visualizing Anomalous Diffusion in Ionic Liquids
10:00 am	*Refreshment Break*	
10:30 am	**John Martinis** *Google Inc./UCSB, Physics*	Quantum Supremacy: Checking a Quantum Computer with a Classical Supercomputer
11:00 am	**Claire McLellan** *UCSB, Physics*	Pushing the Sensitivity of Wide-Field Magnetometry with Nitrogen-Vacancy Center Ensembles In Diamond
11:30 am	**David Hsieh** *Caltech*	Hidden Electronic Phases in Heavy Transition Metal Oxides
12:00 pm	*Lunch*	

Session 4, Thursday Afternoon, February 1, 2018, Corwin Pavilion

1:30 pm	**Matt Helgeson,** **Megan Valentine** *UCSB, Chemical Engineering, Mechanical Engineering*	IRG–3: Resilient Multiphase Soft Materials
2:00 pm	**Francois Barthelat** *McGill University*	Exploring Material Property Space Using Bioinspiration and Microarchitecture
2:30 pm	**Cora Leibig** *Chromatic 3D Materials*	Thermoset Materials for 3D Printing
3:00 pm	*Refreshment Break*	
3:30 pm	**Christine Luscombe** *University of Washington*	Chalcogen Polymers for Nanoparticle Synthesis and Solar Cell Fabrication
4:00 pm	**Xie Zhang** *UCSB, Materials*	Radiative and Non-Radiative Recombination in Hybrid Perovskites
4:30 pm	**Glenn Fredrickson** **Rachel Segalman** *UCSB, Chemical Engineering, Materials*	IRG–2: Polymeric Ionic Liquids
5:00 pm	*Posters and Reception*	

Kerstin Schierle-Arndt studied chemistry at the University of Bonn and received her PhD in 1998 in electrochemistry. She joined BASF in 1998 and was involved in several R&D projects for electrochemical processes for organic and inorganic compounds. After positions within Controlling and Marketing she took over the responsibility for a research group dealing with Inorganic Chemistry as Senior Research Manager in 2007. January, 1st 2018 Kerstin became Vice President Research Inorganic Materials and Inorganic Synthesis. Her research interests are within new or improved materials for electronic and energy applications and she is active in the area of synthesis and process development for inorganic chemicals, reaching from solid state chemistry, nanomaterials through sulfur chemistry up to organometallic chemistry.
In addition she is Associate Director of CARA – California Research Alliance by BASF.

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Francois Barthelat obtained his PhD from Northwestern University in 2006 and is now Professor of Mechanical Engineering at McGill University. At McGill he founded the Laboratory for Advanced Materials and Bioinspiration, with the missions to identify key structures and mechanics of natural materials and to duplicate these features in novel high-performance engineering materials. Dr. Barthelat and his students have discovered new deformation and fracture mechanisms in bone, mollusk shells and fish scales. They have also pioneered new bioinspired materials and systems which they are now implementing in engineering applications: toughened glass for windows and touch screens, flexible scaled armor for industrial gloves, new ceramic composites for bone implants. The new bioinspired strategy he and his students recently developed to toughen glass was selected among the top ten scientific discoveries in Quebec by the magazine *Quebec Science* in 2014. Dr. Barthelat serves on the editorial board of *Scientific Reports*, *Bioinspiration and Biomimetics*, *Journal of the Mechanical Behavior of Biomedical Materials, Experimental Mechanics* and *Applied Mechanics Reviews.*

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Alexandra V. Bayles is a PhD candidate in the Squires and Helgeson labs in the Department of Chemical Engineering at UCSB. Her research interests are in developing tools to better characterize, understand, and ultimately engineer improved soft materials and complex fluids. Alexandra previously attended the University of Delaware, where in 2013 she obtained a BChE with Honors in Chemical Engineering, and minors in Chemistry, Mathematics, and Sustainable Energy Technology. Under the direction of Profs. Eric Furst and Patrick Spicer, she conducted undergraduate research on endoskeletal emulsions, which offer efficient active ingredient delivery in pharmaceuticals, consumer and agricultural products. This work was performed in close collaboration with the Procter & Gamble Co., and was awarded two patents. As an NSF Graduate Research Fellow at UCSB, Alexandra currently uses a novel, microfluidic interferometry platform to study molecular transport in ionic liquid mixtures and ionogels. Improved mechanistic understanding of diffusion in these highly charged materials should enable rational design of task-specific ionic liquids for separation processes, homogeneous catalysis, and electrochemical devices. Alexandra has additionally used differential dynamic microscopy, an emerging Fourier-based analysis technique, to study the dynamics of colloidal and complex fluid motion. During her doctoral work, Alexandra has developed theoretical support for the method and a software package for public distribution.

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Siddharth Dey received his Ph.D. in 2012 from the University of California, Berkeley working with Professor David Schaffer and Professor Adam Arkin. For his post-doctoral research, he moved to Professor Alexander van Oudenaarden's group at the Hubrecht Institute, The Netherlands. In 2017, he moved back to the United States to start his independent research group as an Assistant Professor in the Department of Chemical Engineering at the University of California, Santa Barbara.

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Zvonimir Dogic obtained his B.A. degree in Physics from Brandeis University in 1995, and his Ph.D. from the same university in 2001. Afterwards he spent one year as a Humboldt postdoctoral fellow at Jülich Research Center in Germany, and another year working with the Soft Matter Group at University of Pennsylvania. From 2003-2007 he was a Research Fellow at Rowland Institute at Harvard, after which he joined the Physics Department at Brandeis. In 2017 he moved to the Department of Physics at University of California at Santa Barbara, where he has assumed the Ahlers Chair in Experimental Physics. He was a co-chair of the 2017 Gordon Research Conference on Soft Matter Physics. His research has been recognized by the Cozzarelli prize from the National Academy of Sciences and from 2013 to 2016 he was a Hans-Fisher Senior Visiting Fellow at Technical University of Munich. Dogic's research interests are primarily experimental, and span both equilibrium and non-equilibrium phenomena. Together with his group he uses various biological architectures to create novel soft materials that exhibit physics that is not easily accessible by using purely synthetic methods.

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Doug Fabini is a graduate student in the Materials Department at UC Santa Barbara, working in the lab of Prof. Ram Seshadri. Following his undergraduate work at UC Berkeley in mechanical engineering, Doug dabbled in industry and government before joining UCSB in 2014, including two years on a science and technology policy fellowship at the U. S. Department of Energy. At UCSB, his research has focused on understanding the origins of high performance in main-group halide perovskite photovoltaics, with the goal of discovering more stable, non-toxic alternative materials for optoelectronic applications. His work, which involves both computational and experimental approaches, has focused particularly on elucidating the role of molecular cations and of a proximal lattice instability in directing structure and dictating properties of these curious and promising materials.

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Glenn Fredrickson joined the UCSB faculty in 1990 after having served as a Distinguished Member of the Technical Staff at AT&T Bell Laboratories. The Fredrickson group conducts a broad range of research activities in theoretical and computational polymer science, many of these aimed at understanding self-assembling polymers and complex fluids, and especially block copolymer systems. A computational tool that is unique to the group is the "Field-Theoretic Simulation" technique, which is a numerical procedure for simulating statistical field theory models of complex polymer formulations. The group also maintains strong interactions with experimental teams in academia and industry throughout the world. Glenn is a Member of the National Academy of Engineering, Fellow of American Institute of Chemical Engineers, and Fellow of the American Academy of Arts & Sciences. Recent awards include the Materials Theory Award of the Materials Research Society (2017) and the William H. Walker Award, American Institute of Chemical Engineers (2016).

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Daniel S. Gianola joined the Materials Department at UCSB in early 2016 after holding the positions of Associate Professor and Skirkanich Assistant Professor, all in the Department of Materials Science and Engineering at the University of Pennsylvania. He received a BS degree from the University of Wisconsin-Madison and his PhD degree from Johns Hopkins University. Prior to joining the University of Pennsylvania, Gianola was an Alexander von Humboldt Postdoctoral Fellow at the Forschungszentrum Karlsruhe (now Karlsruhe Institute of Technology) in Germany. Dr. Gianola is the recipient of the National Science Foundation CAREER, Department of Energy Early Career, and TMS Early Career Faculty Fellow awards. His research group at UCSB specializes in research dealing with deformation at the micro- and nanoscale, particularly using *in situ* nanomechanical testing techniques.

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Matt Helgeson is an Assistant Professor in the Department of Chemical Engineering and co-leader of IRG3 on "Resilient Multiphase Soft Materials" in the Materials Research Laboratory at UC Santa Barbara. He received his B.S. in Chemical Engineering at Carnegie Mellon University in 2004, and his Ph.D. in Chemical Engineering at the University of Delaware in 2009. He performed postdoctoral research at MIT before joining the faculty at UCSB. Prof. Helgeson's research focuses on designing and processing complex fluids with well-specified mesostructure, especially those involving colloids (nanoparticles, emulsions, proteins, etc.) in self-assembling & structured liquids. Prof. Helgeson's research has been recognized with a number of awards, including Early Career Awards from both the National Science Foundation (2013) and Department of Energy (2015), a Hellman Foundation Faculty Fellowship (2016), and both the Victor K. LaMer Award (2011) and Unilever Award (2016) from the American Chemical Society.

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Prof. David Hsieh is an experimental condensed matter physicist whose research focuses on macroscopic quantum electronic phases of matter in solid state systems. In particular, Prof. Hsieh is interested in developing novel nonlinear optics, time-resolved ultrafast optics and angle-resolved photoemission-based spectroscopic probes to search for exotic topological and symmetry-broken quantum phases of matter. Prof. Hsieh earned his B.S in Physics and Mathematics from Stanford University in 2003 and his Ph.D. in Physics from Princeton University in 2009 where he worked on both neutron scattering studies of highly frustrated magnets as well as synchrotron-based spin- and angle-resolved photoemission spectroscopy of topological insulators. From 2009 to 2012 Prof. Hsieh was a Pappalardo Postdoctoral Fellow in Physics at MIT. There he developed several table-top laser-based techniques to study the ultrafast opto-electronic properties of topological insulators and wider classes of correlated spin-orbit coupled systems. He joined the Caltech faculty in 2012. Prof. Hsieh is the recipient of a William L. McMillan Award in condensed matter physics, a Sloan Research Fellowship, a Packard Fellowship in Science and Engineering and a Presidential Early Career Award for Scientists & Engineers.

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Dr. Cora Leibig is the founder and CEO of Chromatic 3D Materials, a company focused on developing innovative, disruptive materials for the 3D printing industry. Dr. Leibig has 20 years of professional experience in the materials industry: prior roles include VP of R&D and COO at Segetis, a VC-backed startup company, and Research Director at The Dow Chemical Company. In all of her efforts, she seeks to marry technology innovation with unmet needs in the market, and invest in technology that can accelerate business growth. Cora earned her Ph.D. in Chemical Engineering at the University of California, Santa Barbara in 1997, and her M.S. and B.S. in Chemical Engineering at MIT in 1993. She is married with four children.

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Christine Luscombe grew up in Kobe, Japan. After receiving her Bachelor's degree in Natural Sciences from the University of Cambridge in 2000, she worked with Profs. Andrew Holmes and Wilhelm Huck in the Melville Laboratory of Polymer Synthesis at the University of Cambridge where her research focused on surface modifications using supercritical carbon dioxide for her PhD. She received the Syngenta Award for best organic chemistry project for her PhD. In January 2004, she joined the group of Prof. Jean Fréchet for her post-doctoral studies where she began her research on semiconducting polymers for organic photovoltaics. She was the recipient of the Lindemann Fellowship as well as the Trinity College Junior Research Fellowship (University of Cambridge) for her post-doctoral studies. In September 2006, she joined the Materials Science and Engineering Department at the University of Washington, Seattle. She received a number of young faculty awards including the NSF CAREER Award, DARPA Young Faculty Award, as well as the Sloan Research Fellowship. Her current research focuses on the synthesis of semiconducting polymers for energy applications. She served on the Editorial Advisory Board for Macromolecules and ACS Macro Letters, and is currently serving on the Editorial Advisory Boards for Polymer International, Advanced Electronic Materials, and Journal of Applied Physics. She is an Associate Editor for Journal of Materials Chemistry A, is serving on the IUPAC Polymer Education and Polymer Terminology Subcommittees, and is the Vice President of the IUPAC Polymer Division.

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John Martinis attended U.C. Berkeley from 1976 to 1987. His PhD thesis was a pioneering demonstration of quantum-bit states in superconductors. After postdoctoral research at CEA in France, he joined NIST Boulder where he developed electron counting devices and x-ray microcalorimeters. In 2004 he moved to U.C. Santa Barbara where he continued work on quantum computation. In 2014 he was awarded the London Prize for low-temperature physics research. In 2014 he joined the Google quantum-AI team and heads the hardware effort to build a useful quantum computer.

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Claire McLellan, a native of Virginia, did her undergraduate studies in physics at Wake Forest University in North Carolina. While at WFU she worked with Prof. Oana Jurchescu studying organic small molecules for thin film transistors. Upon arriving to UCSB for graduate school in physics she transitioned into quantum sensing under the tutelage of Prof. Ania Jayich. Alongside members of the Jayich lab, Claire studies the nitrogen vacancy (NV) center in diamond which houses an electronic spin. The NV center is sensitive to magnetic fields, is optically addressable, and operates in ambient conditions, which makes it a suitable magnetometer for biological sensing applications. Claire focuses on integrating ensembles of NV centers for biological sensing and improving sensitivity to probe weak biological magnetic signals. Her talk will focus on the potential of NV centers to non-invasively detect neuron action potentials, the status of the Jayich ensemble magnetometer, and the spin dynamics dominating the NV center ensemble sensitivity.

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Gab Menard joined the Department of Chemistry and Biochemistry at UCSB in 2015. Born and raised in eastern Ontario, Canada, near the nation's capital, Gab first completed his B.Sc. in Chemistry at the University of Ottawa in 2006. He then moved to the west coast of Canada to undertake his M.Sc. at the University of British Columbia in Vancouver working on early metal dinitrogen activation in Prof. Mike Fryzuk's group (2008). Gab then pursued another one of his passions, studying climate change and its impacts by completing a Master's in Environmental Studies (M.E.S.) at York University in Toronto (2010). In 2009, he joined Prof. Doug Stephan's group at the University of Toronto to undertake his Ph.D. studies working on small molecule activation – in particular greenhouse gases – using P/Al-based frustrated Lewis pairs, and finishing up in 2013. Finally, Gab went to the U.S. to pursue his post-doctoral studies in Prof. Ted Betley's group at Harvard University. Here, he gained experience working on first-row transition metal clusters investigating metal-metal communication, high-valent Ni clusters, and small molecule activation.

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Kristin Persson uses atomistic and first-principles computational methods coupled with high-performance computing technology and statistical learning methods to design and improve materials for clean energy production and storage applications. She directs the Materials Project (www.materialsproject.org) which is a multi-institution, multi-national effort to compute the properties of all inorganic materials and provide the data and associated analysis algorithms for every material researcher free of charge. In addition to Science Gateways Community Institute (SGCI) Steering committee, Prof. Persson serves on the US National Academy's Condensed Matter and Materials Research Committee (CMMRC); she is the TMS Materials Genome Initiative Ambassador and recipient of the 2017 TMS Early Career Fellow Award. Furthermore, Prof. Persson has published more than 100 peer-reviewed papers, is the co-founder of Pellion Technologies Inc. and holds several patents in the novel materials for energy storage space. Persson did her academic training at Lund Institute of Technology (Lund, Sweden), the Royal Institute of Technology (Stockholm, Sweden) and the Massachusetts Institute of Technology (Boston, USA). Kristin's research areas are: physics and chemistry of materials; atomistic and first-principles computational methods; high-performance computing technology; clean energy; energy storage; The Materials Project; data analysis algorithms; materials informatics; design of novel materials.

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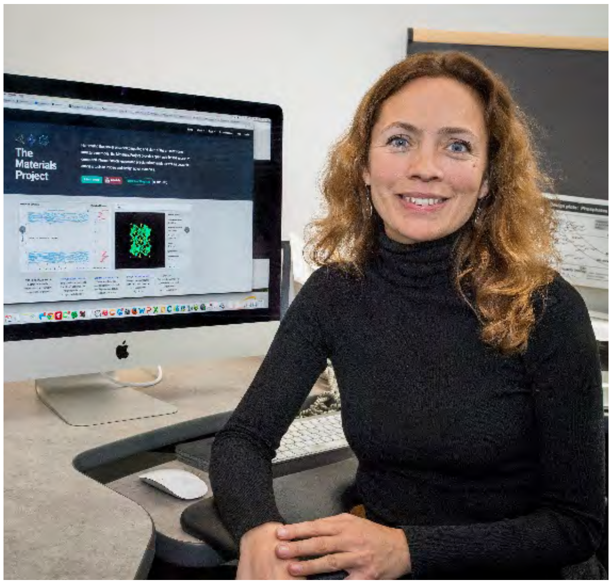

James Rogers, PhD, is Founder and CEO of Apeel Sciences, an agricultural innovation company on a mission to fight food waste and build a sustainable global food supply chain. Dr. Rogers drives corporate strategy and leads Apeel's team of award-winning scientists and engineers who develop products made entirely of plant extracts that double the lifespan of fresh fruit and vegetables. Dr. Rogers received dual undergraduate degrees from Carnegie Mellon University in Materials Science & Engineering and Biomedical Engineering and received his PhD in Materials from the University of California, Santa Barbara. Dr. Rogers was the 2012 recipient of the Frank J. Padden Jr. Award in polymer physics, the premier polymer physics prize in the United States.

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Stuart J. Rowan is currently the Barry L. MacLean Professor of Molecular Engineering and Professor of Chemistry at the University of Chicago, where he moved July 1st 2016. He also has a staff appointment at Argonne National Labs. Prior to this he was the Kent H. Smith Professor of Engineering in the Department of Macromolecular Science and Engineering at Case Western Reserve University. Stuart was born in Edinburgh, Scotland and grew up in Troon, Aryshire on Scotland's west coast. He received his B.Sc. (Hons.) in Chemistry in 1991 from the University of Glasgow and stayed there for graduate school in the laboratory of Dr David D. MacNicol, receiving his Ph.D. in 1995. In 1994 he moved to the Chemistry Department at the University of Cambridge to work with Prof. Jeremy K. M. Sanders FRS. He moved across the Atlantic (and the continental U.S.) to continue his postdoctoral studies with Prof. Sir J. Fraser Stoddart FRS at the University of California, Los Angeles in 1998. In 1999 he was appointed as an Assistant Professor to the Department of Macromolecular Science and Engineering at Case Western Reserve University in Cleveland, Ohio, was promoted to Associate Professor with tenure in 2005 and became a Full Professor in 2008. He is a NSF CAREER awardee, received the Morley Medal (ACS) in 2013, the CWRU Distinguished University Award in 2015, and the Herman Mark Scholar Award (ACS) in 2015. He became an ACS POLY Fellow in 2016 and is a Fellow of the Royal Society of Chemistry. He is Editor-in-Chief of *ACS Macro Letters*, and on the editorial advisory board for the Journal of Polymer Science Part A: Polymer Chemistry, Chemical Science, and J. Macromolecular Sci, Pure & Applied Chem. His research interests include investing the use of dynamic chemistry (covalent and non-covalent) in the construction and properties of structurally dynamic and adaptive polymeric materials. His group works on supramolecular polymers, self-healing materials, stimuli-responsive material and nanocomposites, metal-containing polymers, gels, biomaterials, and developing new synthetic methods for the construction of complex polymeric architectures.

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Morgan W. Schulze earned a B.S. degree in chemical engineering at the University of Texas at Austin and a Ph. D. in chemical engineering from the University of Minnesota, Twin Cities under the guidance of Marc Hillmyer. She is currently a postdoctoral associate working with the Hawker group at the UCSB Materials Research Laboratory where her research focuses on the synthesis and self-assembly of multifunctional polymers.

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Rachel A. Segalman received her B.S. from the University of Texas at Austin and Ph.D from the University of California, Santa Barbara. She was a postdoctoral fellow at the Universite Louis Pasteur before joining the faculty of UC Berkeley and faculty staff member of Lawrence Berkeley National Laboratories from 2004-2014. She also served as the Materials Science Division Director at Lawrence Berkeley National Laboratories from 2013-14. In the summer of 2014, she moved to UC Santa Barbara to be the Kramer Professor of Chemical Engineering and Materials and became Department Chair of Chemical Engineering in 2015. Segalman's group works on controlling the structure and thermodynamics of functional polymers including polymerized ionic liquids and semiconducting and bioinspired polymers. This has led to a host of new and promising applications, particularly in plastic thermoelectrics. Among other awards, Segalman received the 2015 Journal of Polymer Science Innovation Award, the 2012 Dillon Medal from the American Physical Society, the Presidential Early Career Award in Science and Engineering, is an Alfred P. Sloan Fellow and a Camille Dreyfus Teacher Scholar. She is also a Fellow of the American Physical Society and serves on the Board of Directors of the Materials Research Society.

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Megan T. Valentine is an Associate Professor of Mechanical Engineering and Associate Director of the California NanoSystems Institute at UC Santa Barbara, leading an interdisciplinary research group with expertise in biophysics and biomechanics. Current projects range from the investigation of force-sensing and mechanics of vascular and neural tissues to the design of novel bioinspired adhesives and materials. Prior to joining the UCSB faculty in 2008, she completed a postdoctoral fellowship at Stanford University in the Department of Biological Sciences under the support of a Burroughs Wellcome Career Award at the Scientific Interface, and a Damon Runyon Cancer Research Postdoctoral Fellowship. She has won numerous awards, including an NSF CAREER Award, and a prestigious Fulbright Scholar Award to study adhesion mechanics at ESPCI ParisTech in Paris, France. She currently serves on the Executive Committee of the American Physical Society's Division of Biological Physics and is a co-leader of IRG3 on Resilient Multiscale Soft Materials within the UCSB Materials Research Laboratory, an NSF MRSEC.

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Stephen Wilson joined the faculty of the Materials Department at UCSB in 2014. His background is in condensed matter physics and he received his Ph.D. in 2007 from the University of Tennessee, Knoxville. He performed postdoctoral studies at Lawrence Berkeley National Lab from 2007-2009 and served on the faculty of the Physics Department of Boston College from 2010-2014. His current research interests include studies of phase behavior in strongly correlated electron/quantum materials, new states in spin orbit coupled matter, and harnessing many-body electronic states in functional materials. Specific examples include studies of relativistic Mott materials, unconventional superconductivity, quantum criticality, and new approaches to controlling magnetocaloric and cathode materials. Experimental techniques employed in his group include neutron and x-ray scattering, bulk electronic properties characterization (e.g. charge transport, heat capacity, magnetic susceptibility, etc.), and bulk single crystal growth."

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Xie Zhang received his PhD in 2015 from the department of computational materials design at the Max-Planck-Institut für Eisenforschung GmbH (MPIE) and the Ruhr-Universität Bochum in Germany, and continued his research work on structural transformations in high-performance alloys based on first-principles calculations as a postdoctoral researcher till the end of 2016. He joined the group of Prof. Chris Van de Walle at the University of California, Santa Barbara in January 2017. The major focus of his current research work is to quantitatively compute and understand the fundamental radiative and non-radiative recombination processes in hybrid perovskites and other semi-conductors employing newly developed first-principles approaches.

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List of Posters

1. **Cathodes and solid electrolytes for next-generation batteries**, M. B. Preefer, N. S. Schauser, R. A. Segalman, F. Wudl, and R. Seshadri
2. **Coarse-graining polymer field theory for fast and accurate simulations**, J. Liu, K. T. Delaney, and G. H. Fredrickson
3. **Coarsening in the formation of polymer membranes for water filtration**, J. U. M. Garcia, D. R. Tree, K. T. Delaney, and G. H. Fredrickson
4. **Complex cation and anion-modified hybrid perovskite-related materials**, H. Evans, B. Barraza, N. Venkatesan, J. Labram, E. Perry, G. Wu, F. Wudl, M. Chabinyc, and R. Seshadri
5. **Divalent ions modulate macromolecular biological structures**, B. Fletcher, C. Song, P. Kohl, P.J. Chung, H. P. Miller, Y. Li, M.C. Choi, L. Wilson, S.C. Feinstein, and C.R. Safinya
6. ***Endo* and *exo* furan-maleimide adducts: temperature tunable building blocks for efficient polymer modification**, E. H. Discekici, A.H. St. Amant, Ngan Nguyen, I. Lee, C.J. Hawker, and J. Read de Alaniz
7. **Exploration of metal-insulator transitions in AB_4Q_8 defect spinel systems**, J. Zuo, E. Schueller, S. D. Wilson, and R. Seshadri
8. **Exploring quantum criticality in a bilayer magnetic iridate**, Z. Porter, J. L. Schmehr, M. Aling, and S. D. Wilson
9. **Fabrication of polymer-carbon and polymer-ceramic composites through additive manufacturing**, J. E. Regis, L. Chávez, L. Delfin, and Y. Lin
10. **Facile synthesis of miktoarm star polymer by grafting through polymerization**, A. Levi
11. **First-principles calculations on wide-bandgap materials for energy applications**, A. J. E. Rowberg, W. Wang, L. Weston, and C. G. Van de Walle
12. **Geometric control of adhesion inspired by mussel plaque/thread structures,** M. Areyano, L. Gockowski, and M. T. Valentine.
13. **Hydrophobic-mediated assembly of lipid-coated building blocks by double-end anchored polymers**, E. Wonder, C. Liu, K. K. Ewert, P. Kohl, Y. Li, W. Qiao, and C. R. Safinya
14. **Integrating field and particle based simulations to design soft matter materials** , N. Sherck, K. T. Delaney, M. S. Shell, and G. H. Fredrickson
15. **Loss mechanisms in light emitters**, D. Wickramaratne, J.-X. Shen, H. Peelaers, and C. G. Van de Walle
16. **Metal-free visible light-induced growth of polymer brushes under ambient conditions**, B. Narupai, Z. A. Page, N. J. Treat, C. W. Pester, E. H. Discekici, N. D. Dolinski, J. Lawrence, Y. Luo, A. J. McGrath, G. F. Meyers, P. G. Clark, J. Read de Alaniz, and C. J. Hawker
17. **Metamagnetic intermetallics**, E. E. Levin, J. D. Bocarsly, J. H. Grebenkemper, S. Teicher, T. M. Pollock, S. D. Wilson, and R. Seshadri
18. **Multi-material printing in one step with SMaLL (solution mask liquid lithography)**, N. D. Dolinski, Z. A. Page, B. Callaway, F. Eisenreich, R. Garcia, R. Chavez, D. Bothman, S. Hecht, F. Zok, and C. J. Hawker

19. **Optimizing cationic liposome composition for hydrophobic drug loading and delivery to human cancer cells**, V. Steffes, S. MacDonald, M. Murali, K. Ewert, and C. R. Safinya
20. **Polyelectrolyte complexation of conjugated polyelectrolytes for mixed conductive complex fluids**, S. P. O. Danielsen, T.-Q. Nguyen, G. H. Fredrickson, and R. A. Segalman
21. **Resonant inelastic x-ray scattering study of metallic $Sr_3(Ir_{1-x}Rux)_2O_7$**, J. Schmehr, M. Aling, M. Upton, and S. D. Wilson
22. **Role of transition metal identity in dumbbell formation in layered oxide cathode materials**, J. Vinckeviciute, M. D. Radin, and A. Van der Ven
23. **Structural and electronic defects in layered hybrid perovskites**, N. Venkatesan, E. Perry, H. Nakayama, and M. Chabinyc
24. **Structural changes in doped organic semiconductors observed *in operando* using polymeric ionic liquids**, E. M. Thomas, M. A. Brady, H. Nakayama, R. A. Segalman, and M. L. Chabinyc
25. **The determination of globally stable morphologies of block copolymers using particle swarm optimization**, C. L. Tsai, K. T. Delaney, and G. H. Fredrickson
26. **The effect of site-specific tau mutations on microtubule bundle structures**, C. Tchounwou, B. Fletcher, C. Song, P. Kohl, P. Chung, H. P. Miller, Y. Li, M. C. Choi, L. Wilson, S. C. Feinstein, and C. R. Safinya
27. **Tuning block copolymer self-assembly with sequence-defined polypeptoids**, A. Patterson, B. Yu, A. Rosales, and R. A. Segalman
28. **Tuning microbial anaerobic respiration using redox-active conjugated oligoelectrolytes**, S. McCuskey, Z. Rengert, T-Q. Nguyen, and G. Bazan
29. **Understanding the influence of structural distortions on recombination mechanisms in $MAPbI_3$**, J.-X. Shen, X. Zhang, W. Wang, and C. G. Van de Walle
30. **Understanding the nonlinear flow behavior of highly entangled polymer solutions**, M. C. Burroughs, M.E. Helgeson, and L. G. Leal

1. Cathodes and solid electrolytes for next-generation batteries

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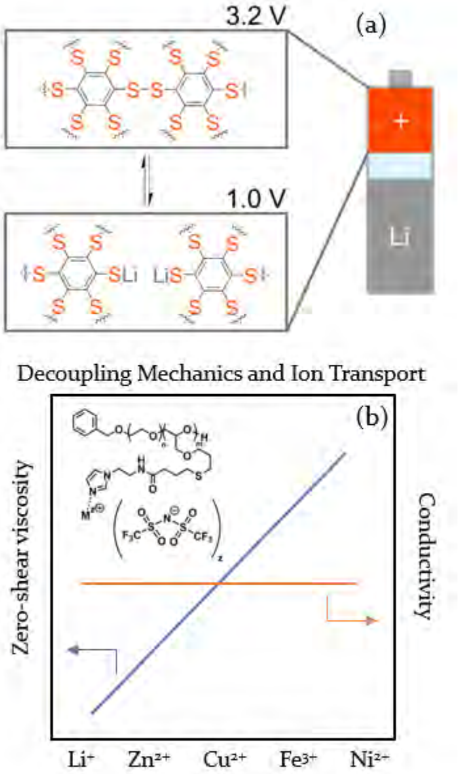
Next-generation battery technologies are crucial for energy independence from fossil fuels because renewable energies such as solar and wind are intermittent. There are many alternatives to current commercialized lithium ion batteries that alter the chemistries and engineering of cathodes, electrolytes, and anodes. The battery team at UCSB presents a combination of ongoing research that specifically targets new cathode and electrolyte materials to improve upon current battery systems.

One research effort focuses on designing novel cathode materials for lithium-sulfur batteries. The main two advantages of Li-S are (i) the high theoretical capacity of elemental sulfur and (ii) the sustainability of sulfur-based materials over toxic, expensive heavy metals such as cobalt. Sulfur can theoretically achieve 1675 mAh g^{-1}, but due to the parasitic polysulfide shuttle problem, the capacity rapidly fades. We present a new sulfur-based material with a theoretical capacity of 609 mAh g^{-1} and 98% capacity retention over 200 cycles.

New electrolyte materials replacing existing organic liquid electrolytes are also needed to improve safety, increase voltage stability, and enable compatibility with new cathode chemistries. Multivalent battery chemistries promise high volumetric energy densities, lower cost and more materials flexibility but are currently limited by the lack of compatible electrolytes. Our project aims to design novel solid-state polymeric electrolytes for the transport of multivalent ions. Initial work has focused on understanding the effect of concentration and ion identity on mechanical properties and conductivity of polymer electrolytes based on metal-ligand coordination. We demonstrate an enhancement in conductivity and mechanical strength at low salt concentrations allowing for the development of rigid ion conducting polymers without the addition of ionically-insulating components.



(a)Disulfide cathode material forms thiolate species upon discharge and crosslinks upon charge to theoretically store 609 mA h g^{-1} in Li-S batteries. (b) Polymer electrolytes based on metal-ligand coordination enable enhanced mechanical properties without hurting ionic conductivity.

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

2. Coarse-graining polymer field theory for fast and accurate simulations

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Phase field mapping is a novel coarse-graining technique for polymer field theories [1] adapted from the force-matching method for particle theories [2]. It uses a complex-valued d+1-dimensional field theory to produce a real-valued d-dimensional field theory that is more computationally efficient to simulate. The mapping can be done from an inexpensive calculation in the fine-grained theory, such as a self-consistent field theoretic (SCFT) simulation [3] in one spatial dimension. The resulting optimized phase field (OPF) model is faster to simulate than SCFT. Compared to previous phase field models, its predictions of structures, length scales and energies are more accurate. The OPF model is also transferable to various types of systems: it can be used to study defect states and different morphologies. Thanks to its combination of speed and accuracy, the OPF model opens up new opportunities for studies in dynamics, in larger systems, and with broader parameter sweeps.

We acknowledge NSF CMMT Grant No. DMR-1506008 and Samsung Electronics for financial support. Computing resources were provided by the Center for Scientific Computing at the CNSI and MRL (an NSF MRSEC, Grant No. DMR-1720256).

Simulations of a defective lamellar structure formed by a diblock copolymer (82 R_{g0} x 82 R_{g0}, where R_{g0} is the unperturbed radius of gyration—approximately 400 nm x 400 nm for PS-b-PMMA), (a) as calculated using SCFT (left); (b) the closest metastable pattern predicted by our optimized phase field model (center); and (c) the closest metastable pattern predicted by the unoptimized Ohta-Kawasaki model (right). Because the optimized phase field model captures the correct lattice spacing for this polymer system, it accurately represents the features shown in SCFT where the Ohta-Kawasaki model fails.

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3. Coarsening in the formation of polymer membranes for water filtration

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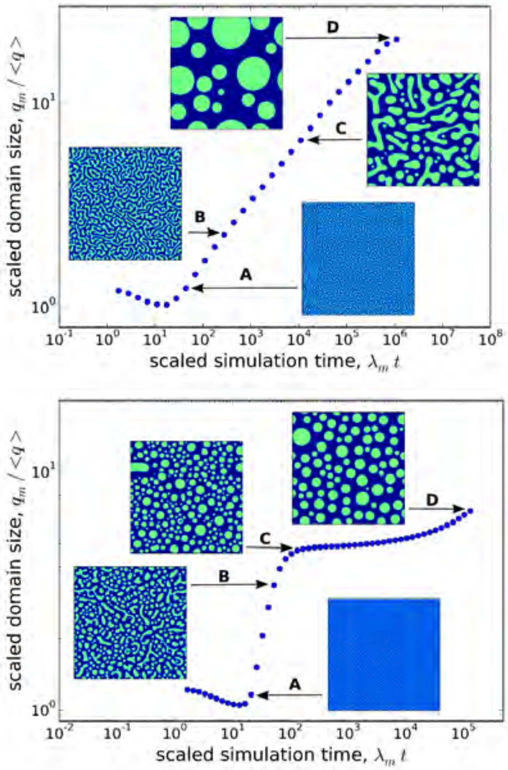
Polymer membranes are essential to providing clean water. Making membranes is a straightforward process: a polymer solution film is immersed in a nonsolvent bath, inducing phase separation and eventual solidification of the film into a membrane. Although simple to implement, the fundamental physics behind this formation process still lacks quantitative explanation. In particular, coarsening plays a major role in determining the bulk morphology of these membranes. In this work, we report the effects of mobility and viscosity contrasts between the solution components (polymer, nonsolvent, solvent) to the coarsening kinetics during the membrane formation process.

We acknowledge support from the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC (DMR-1720256). We also thank Asahi-Kasei Corp. for support. J.U.M.G. acknowledges support from the NSERC PGS-D scholarship program.



Coarsening of the bulk membrane morphology by diffusion (top) and with hydrodynamics (bottom)

4. Complex cation- and anion-modified hybrid perovskite-related materials

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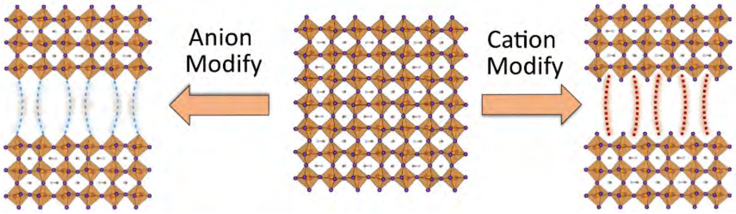
Hybrid perovskite materials (AMX_3, where A = methylammonium or formamidinium, M = Pb, Sn, and X = Cl, Br, I) have attracted considerable attention for their potential use in photovoltaic devices. With impressive experimental device efficiencies comparable to commercialized silicon solar cells, and other attractive qualities such as ease of preparation and use of earth abundant constituent elements, hybrid perovskite compounds promise an exciting chance to improve the efficiency and sustainability of future solar energy. However, these compounds notoriously suffer from ambient environment instability and revert to precursor reagents within hours. This is not an insurmountable problem, and there have been successful efforts in the field to improve the durability of these materials by chemically modifying the perovskite structure to possess hydrophobic regions.[1] This creates a resilient layered 2D material, but one which has 50% less photovoltaic efficiency compared to its 3D counterparts. Our project aims to utilize new chemistry to bridge the gap between reduced photovoltaic performance and increased stability, to produce efficient, low-cost, stable photovoltaic materials. Specifically, we are focused on utilizing functional cationic and anionic organic spacers to create new 2D layered materials.[2]

This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under award number DE-SC-0012541 and facilities supported by NSF DMR 1720256.



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5. Divalent ions modulate macromolecular biological structures

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Divalent ions can mediate condensation of highly charged biological macromolecular assemblies by producing attractions and suppressing repulsions between like-charged structures. Combining small-angle x-ray scattering with x-ray fluorescence techniques has allowed us to directly and quantitatively probe the correlation between the structural transitions of like-charged biomolecules and the density of counterions bound to the supramolecular structures. We report here on the dependence of this attractive electrostatic regime on counterion concentration and type (i.e. ion-specific effects) for two different in vitro systems: tau protein-coated microtubules in dissipative, out-of-equilibrium conditions and DNA molecules confined to two dimensions by cationic liposomes at equilibrium. The functional implications of these ion-mediated transitions in biological assemblies are poorly understood, creating a need for further research.

6. *Endo* and *exo* furan-maleimide adducts: temperature tunable building blocks for highly efficient polymer modification

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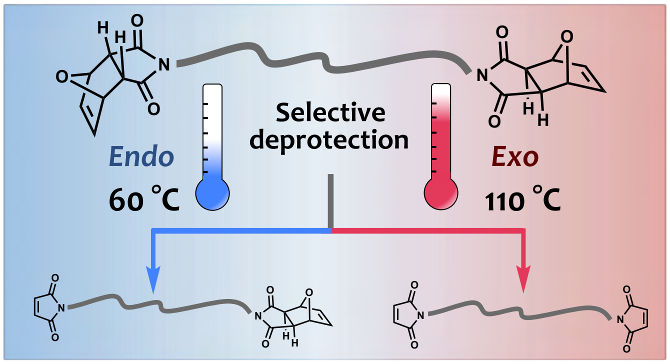
Maleimides exemplify a class of 'click' functionalities that has found widespread utility across the chemical sciences, ranging from antibody development to functional polymer synthesis.[1,2] Traditionally, the high reactivity of maleimides requires the presence of a furan protecting group. To date, only the more thermodynamically stable *exo* isomer has been investigated as a suitable method to introduce reactive maleimides for small molecule and polymer modification. We have identified a set of reaction conditions that enables facile access to scalable quantities of the *endo* isomer, which undergoes deprotection at approximately 50-60 °C. When combined with the *exo* isomer, which deprotects at 100-110 °C, we demonstrate for the first time a powerful approach to selectively and quantitatively introduce reactive maleimides in small molecule and synthetic polymer systems via simple temperature modulation. Furthermore, we simultaneously disclose the first example of incorporating functional maleimides using metal-free atom transfer radical polymerization. We are confident that coupling exceptional synthetic ease with additive-free functional group tunability will facilitate widespread access to increasingly complex functional molecules and create far-reaching synthetic and application-driven opportunities across the chemical sciences.

The research reported herein has been supported in part by the National Science Foundation – Graduate Research Fellowship, the UCSB Graduate Division – Graduate Research Mentorship Fellowship Program and the UCSB MRSEC (NSF DMR 1720256).



Schematic representation depicting temperature tunable functionalization pathways

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7. Exploration of metal-insulator transitions in AB_4Q_8 defect spinel systems

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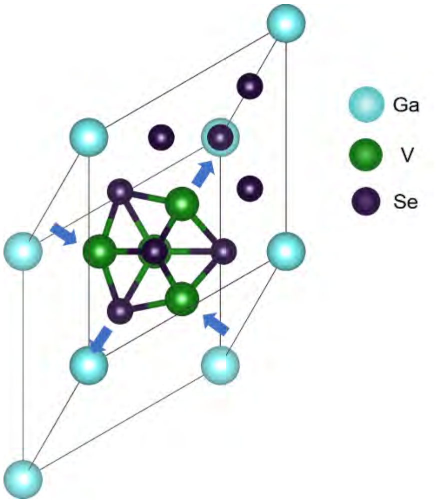

The high temperature *F*–43*m* structure of GaV_4Se_8 with arrows indicating the motions of atoms in the transition to the low temperature *R*3*m* structure.

Materials which undergo a metal-insulator transition — a sudden change in resistivity upon changing temperature, pressure, or composition — have potential for the next generation of electronic switching devices. The underlying mechanisms which drive metal-insulator transitions are of interest both fundamentally in the field of condensed-matter physics and practically for the design of high-performance electronic materials.[1,2] We develop a link between crystal structure and macroscopic electronic properties to realize new metal-insulator transition materials. We start by examining the AB_4Q_8 defect spinel system, where *A* is Al, Ga, or Ge, *B* is Ti, V, Nb, Mo, or Ta, and *Q* is S or Se. These materials, with molecular-orbital-like clusters, start from a cubic *F*–43*m* structure at room temperature and then tend to distort to *R*3*m* or *Imm*2 structures at low temperatures, sometimes accompanied by a metal-insulator transition.[3] By combining theoretical and experimental techniques we examine the interplay between electronic structure, crystal structure, and electronic properties to gain fundamental understanding about the driving forces for metal-insulator transitions in this system. Additionally, compositional control *via* chemical doping provides another tunable parameter to improve our understanding of the relationship between chemistry and electronic and structural properties.

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8. Exploring quantum criticality in a bilayer magnetic iridate

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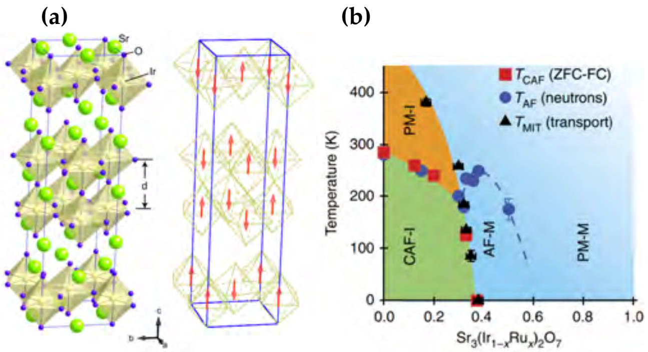
$Sr_3Ir_2O_7$ is a magnetic bilayer system composed of antiferromagnetically (AF) coupled IrO2 layers (Ir^{4+} with J_{eff} =1/2). Below 280K Ir moments order in a G-type AF structure with moments canted slightly away from the long axis. Recent resonant inelastic x-ray scattering studies [1] suggest that Ir ions dimerize across the bilayers with a strong coupling (>90meV magnon gap). Electronically, $Sr_3Ir_2O_7$ is a spin-orbit-assisted Mott insulator. This Mott state is sensitive to perturbation. Upon hole-doping, e.g. by substitution of Ir^{4+} for Ru^{4+}, there is a percolative metal-insulator transition, wherein 1-2 nanometer 'puddles' of $Sr_3Ir_2O_7$ and $Sr_3Ru_2O_7$ remain separated.[2]

Strangely, the Ru-doped system retains AF ordering, like the parent, far past the metal-insulator transition.[2] We speculate that there exists a quantum critical point (QCP) near 60% substitution, a T=0 transition from AF to paramagnetic ordering. If there is a QCP, it is possibly due to quantum fluctuations across bilayers, since it is near the critical concentration for dilute magnetic bilayers.



(a) Nuclear and magnetic structure of $Sr_3Ir_2O_7$; Ir ionic moments (arrows) have G-type antiferromagnetism.[1]
(b) Phase diagram for Ru-doped $Sr_3Ir_2O_7$. Note the metal-insulator transition at x=0.4 for T=0, and the quantum critical point expected near x=0.6.[2]

Here we report electronic transport, calorimetry, and magnetization measurements that investigate the nature of the magnetic phase transition to establish whether there is a QCP. Our preliminary measurements indicate linear temperature dependence of resistivity, a non-Fermi liquid response consistent with 'strange metal' phases near a QCP. These results support continued investigation for novel phases that may exist in this complicated system, which hosts both anisotropic magnetic exchange interactions and considerable electronic correlations.

This work was supported under ARO Award W911NF-16-1-0361. The research reported here made use of shared facilities of the UCSB MRSEC (NSF DMR 1720256), a member of the Materials Research Facilities Network (www.mrfn.org).

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9. Fabrication of polymer-carbon and polymer-ceramic composites through additive manufacturing

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This study presents the fabrication and mechanical characterization of functionalized Multi-Walled Carbon Nanotube (CNT) reinforced photopolymer nanocomposites. In this study we also demonstrate the fabrication of Lead Zirconate Titanate (PZT) embedded photopolymer composites and its dielectric and piezoelectric characterization. CNT was used for its high electrical conductivity as well as its mechanical robustness. Meanwhile, PZT was used due to its high piezoelectric coupling coefficient. The fabrication of composites of this nature through additive manufacturing is a concept that has not been thoroughly explored. In this study, parametric studies were held to find settings that would allow the fabrication of functionalized CNT and PZT nanocomposites through stereolithography (SLA) and digital light processing (DLP) 3D printing processes. In addition, the mechanical properties of functionalized and non-functionalized CNT composites under tensile stress were tested. CNT composites were tested at two different weight percentages in both functionalized and non-functionalized states. Finally, dielectric and piezoelectric properties of the fabricated PZT-photopolymer nanocomposite were studied.

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10. Facile synthesis of miktoarm star polymer by grafting through polymerization

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Miktoarm star polymers are potentially useful in applications ranging from thermoplastic elastomers to drug delivery.[1] In contrast to star homopolymers and radial copolymers, the mikto architecture demands asymmetry in arm connectivity and molar mass distribution, which creates a signficant synthetic challenge. Here, we introduce a new design strategy that simplifies the synthesis of miktoarm star polymers using norbornene-functionalized "macromonomers" and grafting-through copolymerization. Self-assembly in the bulk and dilute solution was studied as a function of molecular composition, arm stoichiometry, and backbone degree of polymerization (*N*). Preliminary insights generated from scattering experiments suggest our materials behave as disperse mikto-star formulations at low *N* with a slow transition to brush-like conformations as *N* increases. These analyses complement previous reports that describe the characterization of star homopolymers using neutron scattering [2] and rheology [3].

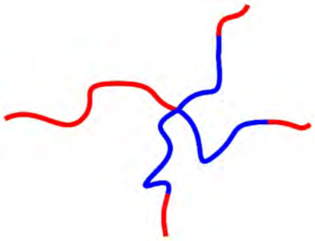
Illustration of a miktoarm star polymer.

This research was supported by the Mellichamp Sustainability Fellowship.

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11. First-principles calculations on wide-bandgap materials for energy applications

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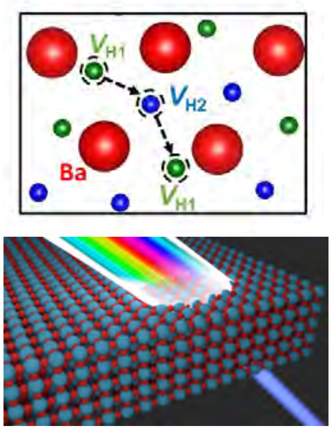
Computational materials science based on first-principles calculations has provided cogent insights into a variety of systems. We present findings on two materials systems with applications in renewable energy technology that illustrate the power and expansiveness of *ab initio* methods.

Interest in renewable sources of energy has contributed to the emergence of hydrogen as a commercial energy source; however, new materials are needed to take full advantage of hydrogen's high energy density. We use first-principles calculations to study the defect properties of the heavy alkaline-earth hydrides (AeH_2; Ae = Ca, Sr, Ba), which have attracted interest as potential hydrogen fuel cell electrolytes thanks to their demonstrated high hydride ion conductivity.[1,2] We find that the migration of positively charged hydrogen vacancies in these materials proceeds with a low energy barrier, suggesting that conductivity can be improved by promoting the formation of these vacancies. We demonstrate that doping these hydrides with alkali metals can lower the vacancy formation energy, providing an engineering solution for improving hydride conductivity.



(a) Schematic depiction of hydrogen vacancy migration in BaH_2.
(b) Artist's rendition of electrochromism, where upon doping only a subset of the incident light is transmitted.

Semiconducting oxides are also attractive for energy efficient applications, including as optical devices. One technologically important oxide is tungsten oxide WO_3, which is a well-known chromogenic material used in smart windows and display technologies. We use first-principles calculations to explore crystalline and disordered structures of WO_3 to demonstrate why these structural changes can enhance absorption at a microscopic level. Our results demonstrate free-carrier absorption as an alternate mechanism for electrochromic behavior. These findings shed light on what electronic features to optimize and engineer for improved functional materials in display technologies.

The research reported in this poster has been supported by DOE, DOD, and NSF. Computational resources were provided in part by the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC (DMR-1720256) and NSF CNS-0960316. A.J.E.R. and W.W. acknowledge funding support from the NSF Graduate Research Fellowship Program (GRFP).

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12. Geometric control of adhesion inspired by mussel plaque/thread structures

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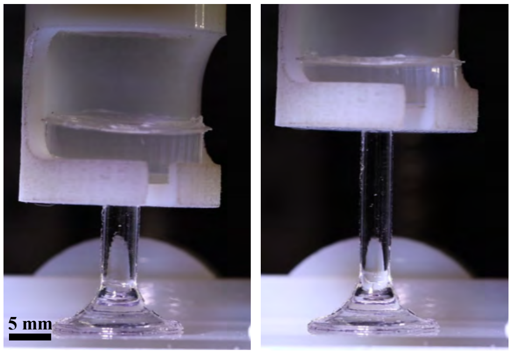

Figure 1 Sample with stalk angle of 90º, loaded at a 90º angle, prior to loading (left), and immediately before delamination (right).

Marine mussel plaque/threads have been long studied for their superb adhesion to a number of substrates including rocks, wood, and metal[1]. They accomplish this without surface pretreatment and under harsh conditions such as rapid loading from predators. Strong adhesion is preserved despite changes in temperature and tidal flows, which alter hydration levels and apply shear loads. Extensive work has been done to understand the chemical dependencies and the role of 3,4-dihydroxy-L-phenylalanine (DOPA) in the mussel's ability to rapidly and strongly bind to surfaces[1,2]. However, many open questions remain regarding the geometrical dependencies and material properties and how these affect adhesion[3,4].

This study seeks to investigate the structural and mechanical origins of the adhesive strength of marine mussel plaque/thread structures via synthetic mimics. We aim to develop a deeper, predictive understanding of how the mussel's properties such as macroscopic geometry impact adhesion. Through the use of custom-designed 3D printed molds, a wide range of shapes and geometries can be quickly manufactured and tested. Experimentally, pull off forces are measured as a function of geometric parameters (Figure 1) including loading angle and the ratio of stalk to contact area radius. The resulting deformation of the structure and the different failure modes (*i.e.* edge vs. center crack initiation) are observed, thereby providing a better understanding of how stresses are dissipated and concentrated throughout the structure.

This work was supported by the NSF MRSEC Program under Award No. DMR 1720256, and made use of the UCSB CNSI Microfluidics Laboratory, and the UCSB Department of Mechanical Engineering's Mechanical Testing Laboratory.

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13. Hydrophobic-mediated assembly of lipid-coated building blocks by double-end anchored polymers

E. Wonder[a], C. Liu[a,b], K. K. Ewert[a], P. Kohl[a], Y. Li[a], W. Qiao[b], and C. R. Safinya[a]
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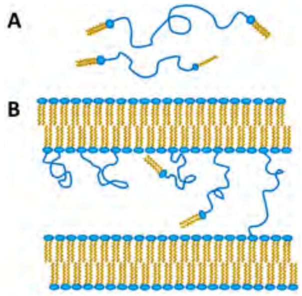
In this work, we introduce PEG (polyethylene glycol) molecules with double-end hydrophobic anchors (DEAs) that allow for hydrophobic-mediated assembly of lipid-coated building blocks. By varying the PEG length, anchor hydrophobicity, and molar fraction of DEA-PEG molecules within a membrane, we can alter the assembly properties of lipid-based systems. This is affected through a change in the equilibrium balance of looping (both anchors in one membrane) and bridging (anchors spanning two membranes) conformations. Using differential interference contrast microscopy, dynamic light scattering, and small angle x-ray scattering, we have demonstrated an ability to tune DEA-PEG-mediated behavior in both pure lipid and lipid–nucleic acid systems.

Cationic liposomes (CLs) are a common synthetic carrier of nucleic acids for gene delivery and silencing. Optimization of DNA delivery and expression requires understanding of the interactions between cellular membranes and CL–nucleic acid nanoparticles (NPs), affecting NP binding, uptake, endocytic trafficking, and endosomal escape. PEGylation is necessary to sterically stabilize the NPs but also has the effect of inhibiting cell-nanoparticle interactions. Adding DEA-PEG molecules to our NPs allows for the formation of polymer bridges between the NP and endosomal membranes. This increases the rate of collisions between the cationic NPs and anionic cellular membranes and promotes membrane fusion and endosomal escape. Confocal imaging of a human prostate cancer cell line (PC3) has shown evidence that NPs modified with DEA-PEG molecules have altered interactions with plasma and endosomal membranes. Colocalization of NPs with recycling (Rab11-GFP) and late endosome/lysosomal (LysoTracker) pathways indicate a change in endosomal trafficking that mimics the effects of very high membrane charge density [1]. This demonstrates the possibility of using DEA-PEG molecules to tune NP-cell membrane interactions in order to promote endosomal escape and exogenous gene expression.



Double-end anchor polymer molecules with PEG linkers and fatty acid anchors (A) bridge two lipid bilayers (B).

This work was supported by the U.S. Department of Energy (DE-FG02-06ER46314), the National Institute of Health (GM-59288) and the National Science Foundation (DMR-1401784). E. W. was supported by the National Science Foundation Graduate Research Fellowship (DGE 1144085). The X-ray diffraction work was carried out both at the Stanford Synchrotron Radiation Lightsource, a Directorate of SLAC National Accelerator Laboratory, and at the shared experimental facilities of the Materials Research Laboratory: an NSF MRSEC, supported by NSFDMR 1121053.

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14. Field and particle based simulations to design soft matter materials

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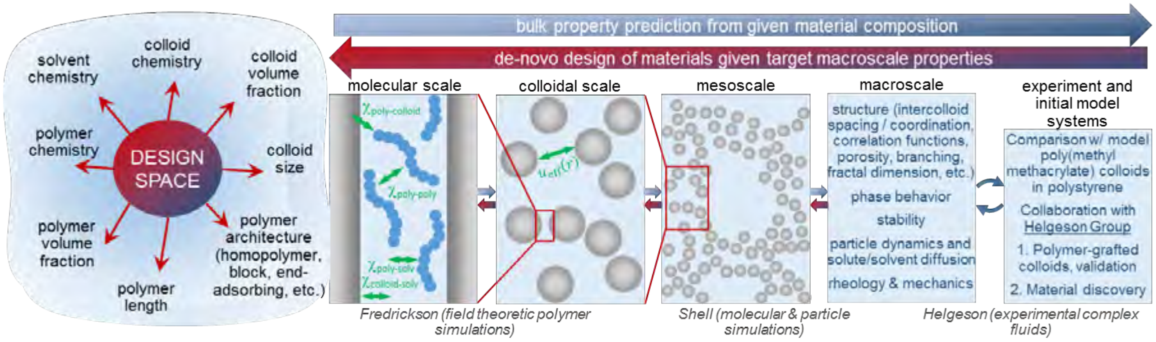
Polymers and colloids are important in a multitude of technologies, ranging from emulsions, foams, dispersions, inks, glues and drilling fluids to drug delivery, cosmetics and food.[1, 2] Colloid-polymer systems also exhibit microstructure resembling biomaterials that have remarkable macroscopic properties; archetypal cases are bones (strength), the feet of mussels (adhesion) and spider silk (workability). Currently, such materials, both in industry and in many labs, are largely designed by trial and error. There exists no systematic design process for engineering or discovering these materials. Truskett and colleagues have recently shown that pair-wise colloidal interactions with long-ranged repulsions and short-ranged attractions can produce a wide array of colloidal microstructures – a previously unexpected result.[3, 4]



Outline of the multiscale computational tool integrating nano- and microscopic scales (right) to mine the large design space (left) for new materials.

Our work couples field theoretic (FT) polymer and colloidal-scale particle simulations, to systematically engineer soft matter materials in-silico combined with experimental validation, (see figure). Specifically, we propose that colloidal microstructure and bulk properties can be engineered using polymers to control colloidal interactions. Polymers are ideal modulators of the colloidal interaction profiles, because they are readily available, cost-effective and highly tunable. This project nucleates a bottom-up and top-down, predictive, computational tool that targets new materials with macroscopic properties like those found in nature, and that seeks to transform industry practice in material discovery and formulation. We acknowledge computational resources from the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC DMR 1720256.

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15. Loss mechanisms in light emitters

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III-nitride alloys are successfully employed in light emitting diodes (LEDs) and laser diodes (LDs) that span the visible spectrum. To enable emerging applications of III-nitride based solid-state lighting which includes adaptive lighting for automobiles, and displays for mobile devices it is essential to establish a microscopic understanding of various loss mechanisms. Experimentally, it is very difficult to discriminate between different sources of loss in optoelectronic devices. We have therefore addressed loss mechanisms in solid-state light emitters using state-of-the-art first-principles calculations.

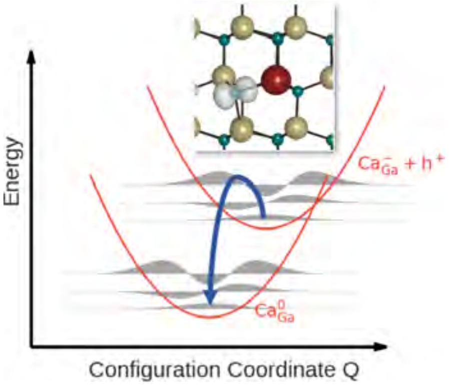

Illustration of nonradiative hole capture into Ca acceptor level in GaN

The presence of point defects and impurities can limit the performance of LEDs by acting as recombination centers through a process known as Shockley-Read-Hall (SRH) recombination. We have identified that the presence of iron, even at concentrations less than parts-per-million in GaN, can be a highly detrimental SRH center [1]. Sources of iron contamination include the stainless steel reactors that are used in some growth techniques for III-nitride semiconductors. Recent experimental work also discovered high concentrations of calcium in the active layer of GaN-based LEDs. The presence of calcium was correlated with a significant reduction in the efficiency of light emission. We find that calcium substituted on the cation site is a strong recombination center, in particular for long-wavelength LEDs operating in the green and yellow region of the spectrum.[2]

Sub-band-gap absorption in the transparent contact of optoelectronic devices can also lead to reductions in efficiency. Transparent conducting oxides such as Ga_2O_3 can be employed as transparent contacts in devices operating in the UV region of the spectrum. We found that for free-carrier concentrations above 10^{19} cm^{-3} strong sub-band-gap absorption can occur in Ga_2O_3 and reduce transparency.[3]

This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award No. DE-SC0010689 and by the National Science Foundation MRSEC program (DMR-1121053).

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16. Metal-free visible light-induced growth of polymer brushes under ambient conditions

B. Narupai[a,b], Z. A. Page[b], N. J. Treat[b], C. W. Pester[b], E. H. Discekici[a,b], N. D. Dolinski[b], J. Lawrence[b], Y. Luo[b], A. J. McGrath[b], G. F. Meyers [c], P. G. Clark[c], J. Read de Alaniz[a] and C. J. Hawker[a,b]
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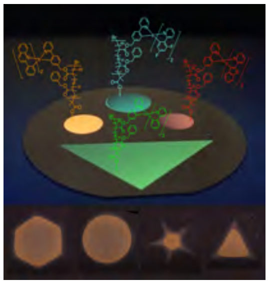
[c]The Dow Chemical Company, Midland, MI 48667

A facile grafting-from methodology that uses light to grow polymer brushes under ambient conditions is reported. Using metal-free atom transfer radical polymerization, *N*-phenyl phenothiazine was found to act as both an oxygen scavenger and photocatalyst, where growth only occurs in oxygen diffusion-limited regions underneath a cover slip. This allows for excellent spatial and temporal control of brush growth from minimal reaction volumes. The preparation of well-defined brush patterns, tetrablock copolymers, and emissive brushes from precious metals over large surface areas demonstrate the practicality and versatility of the presented platform.



The excellent spatiotemporal control of brush growth under ambient conditions over large surface areas via light-mediated metal-free atom transfer radical polymerization.

We thank the MRSEC program of the National Science Foundation (DMR-1720256) and the Dow Chemical Company through the Dow Materials Institute at UCSB for financial support.

17. Metamagnetic intermetallics

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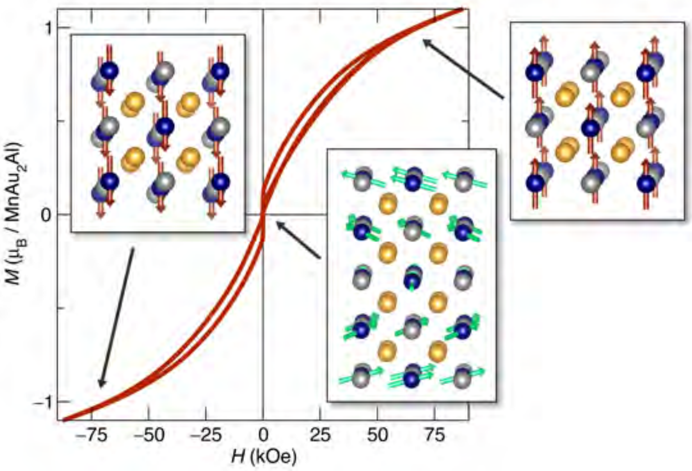
Some magnetic materials can display a dramatic change in magnetic structure upon application of a magnetic field. This property, known as metamagnetism, is promising for a variety of applications including next-generation spintronics, efficient magnetic refrigeration and thermomagnetic electricity generation. Metamagnetic transitions can take many forms, including spin-reorientations from antiferromagnetic to ferromagnetic order, transitions or crossovers from a nonmagnetic state to a magnetic state, or topological transitions between incommensurate chiral states. Of particular interest are materials with metamagnetic transitions that couple to structural or electronic phase transitions. Here, we present magnetic measurements, X-ray and neutron diffraction experiments, and density functional theory calculations on some intermetallic phases that show striking metamagnetic phenomena. We focus on the chemical crystal structures of the materials and how they influence the magnetic properties, including through spin-orbit coupling and the magnetostructural interaction.

This work was supported by the MRSEC Program of the National Science Foundation (NSF) under Award No. DMR 170256.



(a) Schematic of a possible model of metamagnetism in the Heusler intermetallic $MnAu_2Al$. At zero field, spin-orbit coupling causes the atomic spins to form a spiral. As a magnetic field is applied, the spins cant towards the direction of the applied field.

18. Multi-material printing in one step with SMaLL (solution mask liquid lithography)

N. D. Dolinski[a,b], Z. Page[b], B. Callaway[a], F. Eisenreich[b,c], R. Garcia[b], R. Chavez[b], D. Bothman[d], S. Hecht[c], F. Zok[a], and C. J. Hawker[a,b]
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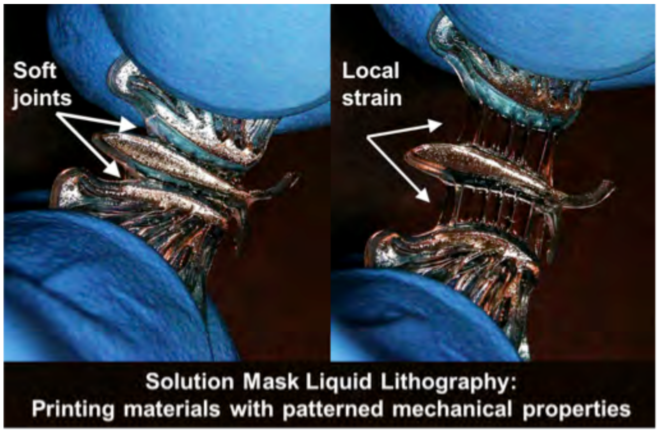

A 'butterfly' material printed using Solution Mask Liquid Lithography with soft joints that undergo local strain under tensile loading.

The ability to rapidly produce parts from digital designs through 3D printing has led to tremendous breakthroughs in scientific discovery and manufacturing.[1] Recently, new 3D printing methods capable of distributing multiple material stocks spatially have enabled the patterning of so-called multi-material parts. Multi-material parts have a unique ability to mimic natural systems, that often take advantage of interlocking domains of soft and hard materials, giving access to highly engineered materials properties.[2] However, current multi-material printing techniques utilize traditional layer-by-layer printing systems, leading to end products with undesirable defects and hindered properties.[1] To address this, we developed a novel multi-material printing technique, enabled by photochromic dyes, to rapidly produce layerless structures with patterned mechanical / chemical properties. To demonstrate the flexibility and utility of this technique, several bioinspired motifs were produced, exhibiting programmable response and enhanced properties.

This work was supported by the Institute for Collaborative Bio-technologies through grant W911NF-09-0001 from the U.S. Army Research Office. The content of the information does not necessarily reflect the position or the policy of the Government, and no official endorsement should be inferred.

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19. Optimizing cationic liposome composition for hydrophobic drug loading and delivery to human cancer cells

V. Steffes[a], S. MacDonald[a], M. Murali[a], K. Ewert[a], and C. R. Safinya[a]
[a]University of California, Santa Barbara, CA 93106

Paclitaxel (PTXL) is a hydrophobic drug that acts as a mitotic inhibitor, inducing apoptosis and halting the proliferation of tumor cells. PTXL is most often administered in hospitals in the patented formulation Taxol® whose solvents cause hypersensitivity reactions in addition to the side-effects of the chemotherapeutic PTXL drug. To improve the therapeutic efficacy of PTXL, it should be administered by a non-toxic delivery agent with tumor cell specificity. Lipid nanoparticles have many advantages as drug delivery vehicles including a diverse set of lipid building blocks to tune physical and chemical properties, low toxicity, and their ease of modular processing. Our recent study [1] revealed that loading PTXL in cationic liposomes (CLs) at a concentration lower than the membrane solubility limit (< 3 mol%) may have short and long-term benefits for drug delivery outcomes compared to the CL formulation EndoTAG®, which employs CLs at the PTXL membrane solubility limit. In the work presented here, we consider the effects of lipid curvature, hydrophobic tail saturation, and inclusion of PEG-lipid on PTXL solubility in CLs, and we correlate the physical properties of the liposomes to PTXL delivery efficacy observed in *in vitro* cell studies.

V. S. acknowledges support from the National Science Foundation's Graduate Research Fellowship program under Grant No. DGE 1144085.

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20. Polyelectrolyte complexation of conjugated polyelectrolytes for mixed conductive complex fluids

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Electrostatic assembly strategies of conjugated polyelectrolytes, which combine a π-conjugated polymer backbone with pendant ionic groups, offer an opportunity for tuning materials properties and device performance. Herein, the polyelectrolyte complexation behavior of a cationic conjugated polyelectrolyte (Poly{3-[6-(1-butylimidazolium-3yl)hexyl]thiophene-2,5-diyl bromide}) with polystyrene sulfonate, is explored to illustrate an equilibrium phase diagram, Fig. 1, parametrized by electrostatic strength, solvent quality, polymer concentration. Four distinct phases are formed: soluble complexes, precipitates, complex coacervates, and gel precipitates. Each phase has unique local structure and organization, which translates to phase-dependent conductivity and electronic properties.

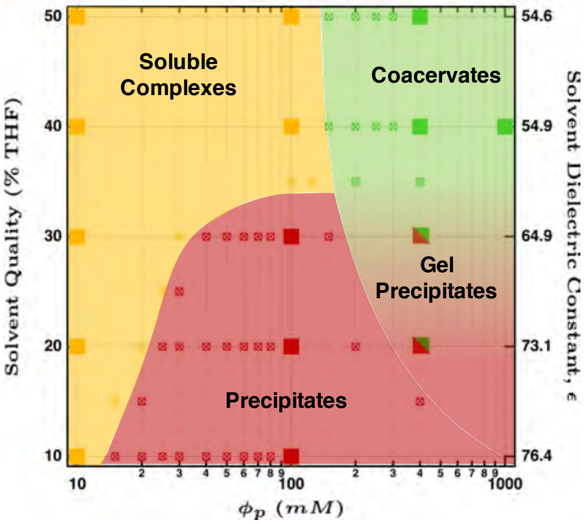

Figure 1. Equilibrium Phase Diagram of P3BImHT+PSS Polyelectrolyte Complexes.

21. Resonant inelastic x-ray scattering study of metallic $Sr_3(Ir_{1-x}Ru_x)_2O_7$

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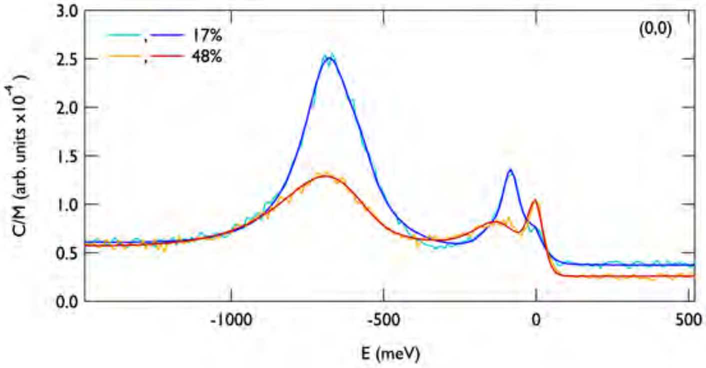
[c]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439

$Sr_3Ir_2O_7$ is a strongly-correlated J_{eff}=1/2 Mott insulator which is extremely susceptible to perturbation by chemical substitution. Doping with Ru on the B-site leads to a percolative metal-insulator transition near 33% Ru-substitution, but antiferromagnetic order persists well into the metallic phase with a pronounced maximum of TN around 45% doping[1]. Here we report resonant inelastic x-ray scattering results on Ru-doped Sr327 samples within the metallic antiferromagnetic regime. We observe that spin wave excitations reminiscent of the undoped parent compound survive well into the metallic phase. The bandwidth is reduced as expected for the case where disorder quenches longer-range exchange interactions, but interestingly the excitation gap is strongly increased, from around 90 meV for the undoped parent up to 125 meV for 48% Ru-substitution. Potential explanations for this behavior are discussed.

We acknowledge funding through NSF DMR 1720256 and ARO.



Representative RIXS spectra upon Ru-doping of $Sr_3Ir_2O_7$

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22. Role of transition metal identity in dumbbell formation in layered oxide cathode materials

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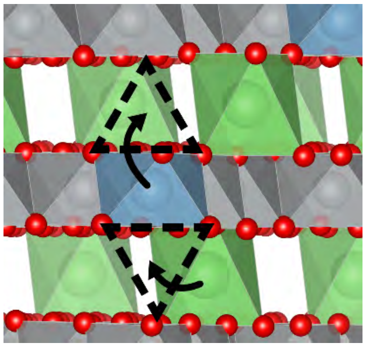
Materials Department, University of California, Santa Barbara, CA 93106

Li-ion batteries suffer greatly from degradation when charged and discharged over many cycles.[1] This is partly due to the layered material transforming into spinel or rock salt structures. The transformation occurs when atoms move between layers, hopping from octahedral sites in the transition-metal layer to tetrahedral sites in the Li layer and onto other sites after that. Limiting this migration could result in longer lifetimes for batteries. Often, the energy for migration of atoms across layers is attributed to the species that is moving. However, our calculations suggest that the local environment of the migrating atom can be just as significant, which we analyze by exploring the electronic structure of layered CoO_2, NiO_2, and MnO_2. We show that certain transition-metals like Ni may aid in suppressing interlayer atom migration. However, the underlying principles of our analysis can be applied to other systems where defect formation is of interest.



Dumbbell formation is affected by both the identity of the migrating atoms and their local environment.

The research reported has been funded in part by the National Science Foundation, Grant DMR-1410242. We acknowledge support from the Center for Scientific Computing from the CNSI, MRL, NSF MRSEC (DMR-1121053), and HewlettPackard. This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. The work was also supported as part of the NorthEast Center for Chemical Energy Storage (NECCES), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DESC0012583.

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23. Structural and electronic defects in layered hybrid perovskites

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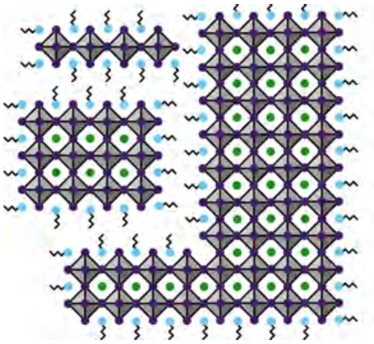
Solution-processable, hybrid halide Ruddlesden-Popper (R-P) phases have favorable electronic properties with increased stability relative to their 3D counterparts ($CH_3NH_3PbI_3$). Although layer confinement from the introduction of larger, organic cations leads to anisotropic charge transport, our previous work shows that the in-plane mobility of single-layer Pb-I perovskite sheets is comparable to $CH_3NH_3PbI_3$ [1], making control over thin-film structure essential to device performance. Here we study R-P compounds with an *n*-butylammonium cation, $(BA)_2(MA)_{n-1}Pb_nI_{3n+1}$, with varying thickness of Pb-I perovskite sheets. Specular diffraction shows a gradual change in thin-film texture with increasing *n*, with the Pb-I sheets changing from parallel to perpendicular with respect to the substrate [2]; however, in-plane disorder is apparent from grazing-incidence diffraction. Additionally, time-resolved microwave conductivity (TRMC) measurements show smaller yield-mobility products and carrier lifetimes than in $CH_3NH_3PbI_3$ [2]. Most interestingly, external quantum efficiency measurements of solar cells formed with these materials show sharp absorption edges despite structural disorder. From this, we conclude that these R-P phases have a high electronic defect tolerance and their performance is related to the alignment of the layers relative to the direction of transport.


Proposed structure of *n* = 4 Ruddlesden–Popper thin films, showing intergrowth of lower layer thicknesses.

Development of the microwave conductivity instrument was supported by the Defense Threat Reduction Agency under award number HDTRA1-15-1-0023. Materials synthesis and characterization was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under award number DE-SC-0012541. The research reported here made use of shared facilities of the UCSB MRSEC (NSF DMR 1720256), a member of the Materials Research Facilities Network (www.mrfn.org). J. G. L. gratefully acknowledges Virgil Elings and Betty Elings Wells for financial support through the Elings Fellowship Awards.

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24. Structural changes in doped organic semiconductors observed *in operando* using polymeric ionic liquids

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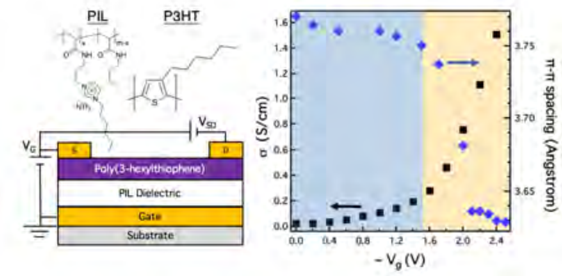
[b]Lawrence Berkeley National Laboratory, Berkeley, CA 94720
[c] Department of Chemical Engineering, University of California, Santa Barbara, CA 93106

The effect of structural variations on charge transport is often overlooked in electrically doped organic semiconductors. In order to increase their electrical conductivity, charge carriers are introduced into conjugated polymers by extrinsic dopants, usually by introduction from solution or by infiltration from a vapor. Frequently, electrical conductivity is modeled using a static density of states filled with carriers, but it is important to consider changes in microstructure as carrier concentration increases to the point that the dopant (or counter-ion) is at a comparable level to the sites in the semiconductor.



A correlation between electrical conductivity, σ, and spacing between π faces in the semiconductor P3HT gated in an electrochemical transistor.

We have explored the structural evolution of poly(3-hexylthiophene), a p-type organic semiconductor, in a thin-film transistor (TFT) configuration using a polymeric ionic liquid (PIL) gate dielectric. PILs contain one ion covalently bonded to the polymer backbone and one ion that is mobile, which allows for control of counter-ion diffusion as well as low-voltage device operation. Through the use of *in operando* grazing incidence wide-angle X-ray scattering (GIWAXS), we can directly measure changes in microstructure as a function of applied gate bias in real-time. We observe that changes in semiconductor domain structure are highly dependent on the sign and magnitude of the applied gate voltage; bias less than |1.6| V do not lead to any change in microstructure, while bias larger than |1.6| V results in swelling of polymer crystallites due to ion infiltration. For the voltage range explored, out-of-plane ("alkyl") stacking distances within the crystalline regions increased by more than 12%, while the distance between π-stacks decreased by approximately 4%. There is a commensurate increase from 5 x 10–3 S cm–1 to greater than 10 S cm–1 in electrical conductivity of P3HT at high doping levels. Shifts in microstructure are irreversible at high bias, a clear indication of permanent changes in crystalline ordering in the high carrier concentration regime. This work indicates that substantial differences exist between a doped polymer and its insulating state, signifying the importance of incorporating doping-induced disorder into charge transport models for organic semiconductors.

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25. The determination of globally stable morphologies of block copolymers using particle swarm optimization and self-consistent field theory

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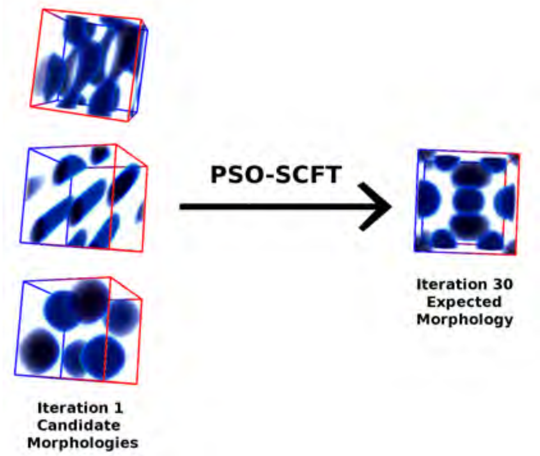
The unguided search for the stable phase of a block copolymer of a given composition and architecture is a problem of global optimization with important ramifications from a materials discovery perspective. In this poster, we present the development of a reciprocal-space Particle Swarm Optimization (PSO)-SCFT method in which we manipulate the Fourier components of SCFT fields near the principal shell. Effectively, the PSO facilitates the search through a space of reciprocal-space SCFT seeds which yield a variety of morphologies. We present results for applying PSO-SCFT to diblock and miktoarm copolymers, and discuss the successes and challenges of the method.



PSO-SCFT applied to AB_4 miktoarm with the successful recovery of the expected, globally stable A_{15} morphology

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26. The effect of site-specific tau mutations on microtubule bundle structures

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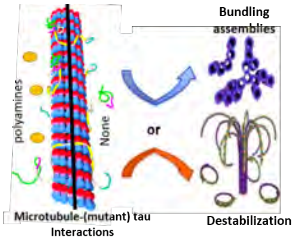
Microtubules (MTs) are biological nanostructures that exhibit GTP-hydrolysis controlled polymerization-depolymerization transitions which enable many important cellular functions. In neuronal axons, inherently dynamic MT architectures are functionalized by binding of the MT-associated phosphoprotein tau.[1] Changes in MT-tau associations have been noted in the literature as a consequence of post-translational modifications to tau such as hyperphosphorylation leading to the hallmarks of several neurodegenerative disease states. [2] We hypothesize that post-translational alterations to specific residues in close proximity to the MT-binding region of tau may influence how tau mediates MT architectures in axons. Furthermore, we demonstrate that purification of site-specific mutagenic tau is now readily achievable with expression of mutant recombinant tau containing a poly-His-tag.[3] Similar to phosphoprotein tau, we have previously reported [4] that biologically relevant polyamines such as spermine also directly modulate electrostatic interactions between MTs leading to unique bundling architectures. Here we probe dynamical MT bundling architectures in the presence of site-specific mutagenic tau with and without polyamines using transmission electron microscopy (TEM) and small angle x-ray scattering (SAXS).



MT bundling architecture in the presence of site-specific mutagenic tau with and without polyamines.

This research is supported by grants from the Department of Energy (DOE), the National Institutes of Health (NIH), and the National Science Foundation (NSF).

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27. Tuning block copolymer self-assembly with sequence-defined polypeptoids

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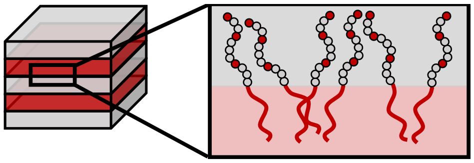

Block copolymer assembly into ordered microdomains is affected by comonomer composition and sequence.

Polymer materials that contain two or more distinct chemistries will phase separate unless covalently attached, and bonded copolymers of different chemical blocks self-assemble into ordered microdomains in order to minimize their mixing energy. Block copolymers with tunable compatibility enable direct control over segregation strength, a key driving force for self-assembly. The miscibility between blocks of an AB copolymer is increased by incorporating B-like units into the A block, and while tapered profiles from semibatch methods have shown compatibilizing effects, fully sequence-defined polymers offer a unique opportunity to control both the composition and distribution of comonomers. We have synthesized polypeptoid–polystyrene diblock copolymers, where the polypeptoid block has styrene-like units precisely incorporated with ether comonomers via high-yielding solid-phase synthesis. First, as styrene-like groups are added to the polypeptoid, the order–disorder transitions (ODTs) are lowered by more than 30 °C. Following this, compatibilizing units are incorporated in different sequences, such as tapered from the block junction or distributed evenly. Within this set of materials with identical composition but different sequence, the ODTs vary by 15 °C. It is expected that sequence affects the effective interaction parameter, chi, which can be quantified using interfacial segregation. These studies demonstrate the ability for sequence control to tune the phase stability of self-assembling block copolymers.

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28. Tuning bacterial anaerobic respiration using redox-active conjugated oligoelectrolytes

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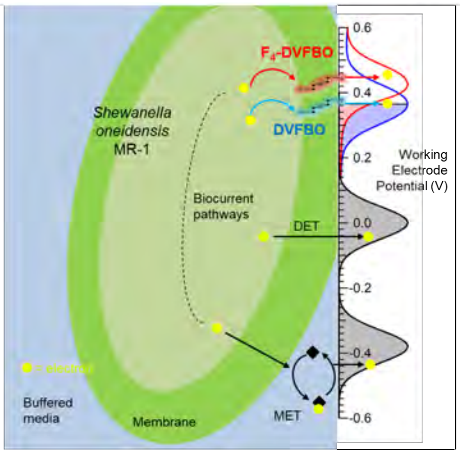
Insertion of artificial constructs into the membrane of microorganisms can increase their ability to electronically communicate with abiotic components and is therefore of interest in bioelectrochemical technologies. One set of relevant molecular systems known as conjugated oligoelectrolytes (COEs) contains an electronically delocalized backbone bearing ionic functional groups [1,2]. Redox-active COEs were recently designed to mimic the function of native membrane proteins that move electrons through iron-containing cytochromes [3]. We present a new redox-active COE called DVFBO that has a π-delocalized core capped on each end by ferrocene units. Fluorination of the core (F4-DVFBO) produces a COE with similar optical properties, membrane affinity, and toxicity, but results in a higher oxidation potential (427 mV compared to 365 mV vs Ag/AgCl). These redox-active molecules were added to anaerobic microbial three-electrode electrochemical cells (M3Cs) containing *Shewanella oneidensis* MR-1 to evaluate their ability to participate in biocatalytic current production. In M3Cs poised at 200 mV, negligible current enhancement is seen compared to controls. However, at 365 mV, DVFBO increases steady-state biocurrent from S. oneidensis by 67 ± 12% relative to controls while F4-DVFBO only increases biocurrent by 30 ± 5%. Cyclic voltammetry supports that DVFBO is the primary conduit of the increased current in reactors and F4-DVFBO has less activity at the lower poised potential. The overall impact is the ability to modulate electron transfer from microbial species via the oxidation potential of the COE.



The oxidation potential of membrane-intercalating DVFBO and F4-DVFBO modulates electron extraction.

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

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29. Understanding the influence of structural distortions on recombination mechanisms in $MAPbI_3$

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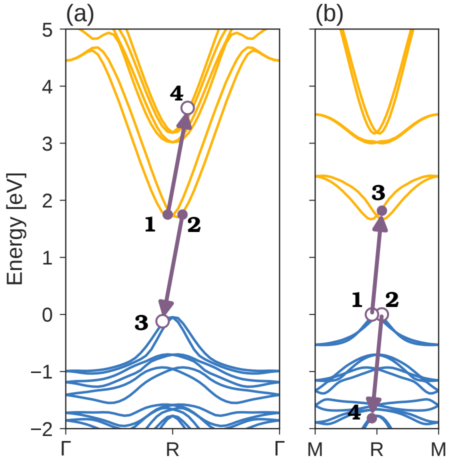
Hybrid perovskites have generated tremendous attention recently due to their excellent solar-conversion efficiency (>22%).[1] Accurate modeling of solar cells requires an understanding of the radiative recombination process. With such a high solar-conversion efficiency, detailed balance in the Shockley-Queisser formulation also suggests that hybrid perovskites are useful for light-emitting diodes (LEDs). The operation of LEDs requires high carrier densities, typically greater than 10^{18} cm^{-3}, compared to photovoltaics where the carrier density is fundamentally limited by the availability of solar radiation. In this regime, Auger recombination (which is proportional to the third power of the carrier density) can lead to significant efficiency loss in the material.

We focus on the prototypical hybrid perovskite, $CH_3NH_3PbI_3$ ($MAPbI_3$). A fundamental feature of the electronic structure of $MAPbI_3$ is the dramatic effects of spin-orbit splitting at the band edges of the material. Using a fully first-principles treatment of the electronic structure and the spin-orbit effects, we simulate the radiative and Auger recombination processes in MAPbI3. For the radiative process, contrary to other proposed models [2], we demonstrate that the band extrema have similar spin orientation and their slight momentum mismatch has only a minor impact on the radiative recombination rate. Our calculated radiative recombination coefficient is in agreement with experimental values and of similar magnitude compared to typical direct-gap semiconductors. For the Auger process, we find that $MAPbI_3$ has a very high Auger recombination coefficient, around two orders of magnitude higher than III-V semiconductors with similar band gaps. We also examine the influence that cation replacement and the orientation of the MA molecule have on these recombination mechanisms.



Band structure of $MAPbI_3$ along the Γ → R and M → R directions. Individual Auger recombination events are indicated by the arrows

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30. Understanding the nonlinear flow behavior of highly entangled polymer solutions

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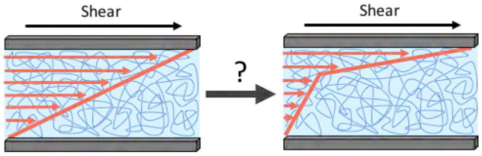
A central goal in the field of polymer processing is to develop constitutive models that relate how microscopic structure of entangled polymers contributes to the observed macroscopic stress in highly nonlinear flows. Although conventional polymer constitutive models have been demonstrated to fit transient and steady shear rheology data, experiments have revealed a wealth of complex phenomena under shearing flow that are not predicted by the models, and are yet highly problematic in conventional polymer processing. These include wall slip, secondary flows, and, most controversially, shear banding. Similar to banding in metals, the latter involves the separation of flow into two or more regions of distinct shear rate. If present, these complications invalidate the central assumption of uniform shearing typically assumed in conventional rheological models. By contrast, recent 1D flow simulations [1] that couple the flow to nonhomogeneous polymer concentration fields have found that shear-induced demixing in polymer solutions could explain many of these phenomena, where bands of different local shear rate coincide with regions of significantly different local polymer concentration. To date, there is a lack of experimental data that would allow for validation and refinement of these new nonhomogeneous constitutive models.



Entangled polymer solutions can exhibit complex phenomena in shear flow that is not predicted by conventional constitutive models

As a first step towards such experiments, we report efforts to eliminate wall slip and secondary flows in order to affirm the existence of shear banding in entangled polymer solutions. To do this, we use rheo-particle tracking velocimetry (rheo-PTV) to quantify the flow field of entangled solutions of polystyrene. We have found that highly entangled polymer solutions (> 30 entanglements per chain) exhibit strong wall slip on glass surfaces, but wall slip is significantly reduced when the glass surface is covered with a PET film. Interestingly, we find the observed transient shear stress to be qualitatively similar with and without wall slip, but much different quantitatively. This highlights the importance of performing simultaneous rheological and flow visualization measurements, and calls into question the accuracy of previous comparisons of rheological data with conventional constitutive models. Additionally, we observe anomalous velocity profiles in highly entangled solutions when there is a free surface of the fluid under shear. The observed velocity profiles are believed to be indicative of secondary flow resulting from edge fracture of the air-fluid interface. We discuss various solutions to eliminate the edge fracture instability. *In situ* small angle light scattering experiments performed under flow confirm that a second overshoot in the transient shear stress is indicative of large-scale demixing of polymer in solution. This second overshoot depends on temperature, concentration, and flow strength as expected from the flow-concentration coupling model. This work has established experimental techniques to enable reliable measurements of highly entangled polymer solutions, and suggests that shear-enhanced concentration fluctuations provide a means by which to explain the flow instability of shear banding in highly entangled polymer solutions. This work has been supported by the National Science Foundation under award number CBET-1510333.

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