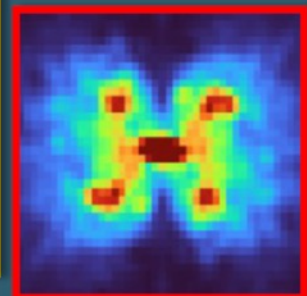
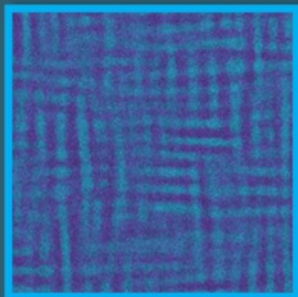




Materials Research Science and Engineering Center University of California Santa Barbara

NSF DMR 1720256
Annual Report 2021 – 2022



UC SANTA BARBARA
MRL
Materials Research Laboratory
NSF Materials Research Science and Engineering Center [DMR 1720256]

National Science Foundation
NSF **M** **R** **S** **E** **C**
MATERIALS RESEARCH SCIENCE AND
ENGINEERING CENTERS

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1 EXECUTIVE SUMMARY

1A. Vision and Overview

The UC Santa Barbara MRSEC recognizes that materials research is inherently interdisciplinary, and that major advances require expert input from multiple domains. In addition, advanced materials research is resource-intensive. Unraveling the details of structure and function to develop the fundamental understanding required for advancing the next generation of useful materials necessitates the use of multiple characterization and measurement tools, coupled with theory and high-performance computation. The central role of the UC Santa Barbara MRSEC is to sustain the necessary collaborative research and training infrastructure that drives a portfolio of transformative materials research. Inherent to the UC Santa Barbara MRSEC goals is a desire to be highly inclusive, and involve a broad range of committed participants. Senior investigators drawn from several disciplines work collectively toward outcomes that would not emerge without their collective inputs. Equal in emphasis to advancing the research goals, the MRSEC trains and nurtures a diverse group of future leaders in materials research. Fulfilling our educational goals requires being able to prepare researchers with the skills required for the modern technical workforce. Stakeholders in the functioning and success of the MRSEC include K–12 students and teachers, undergraduate research interns, graduate student and postdoctoral researchers, faculty investigators, facility users from outside the MRSEC, start-up and established industry partners, and collaborators in the US and abroad. To accomplish the vision of the MRSEC, the leadership and participating senior investigators pay close attention to the three key components that are crucial to a successful MRSEC, notably IRG and Seed (as well as iSuperSeed) research, Education and Outreach, and Shared Experimental Facilities (SEFs), ensuring that they work in a synergistic and integrative manner.

Current MRSEC Research: The three Interdisciplinary Research Groups (IRGs) address problems in materials research whose solutions require collaborative input from multiple dedicated teams of interdisciplinary researchers. Every IRG develops innovative approaches to every aspect of the materials research work-flow that is based around synthesis and processing, theory and computation, and characterization and measurement/testing. These different aspects are devised to work seamlessly to drive advances across a range of functional materials classes. The three IRGs, **IRG-1: Magnetic Intermetallic Mesostructures**, **IRG-2: Polymeric Ionic Liquids**, and **IRG-3: Resilient Multiphase Soft Materials**, trace an arc from hard magnetic intermetallic materials and their microstructure, to chemistry and engineering of an underexplored class of polymeric materials, to biomaterials, and bio-inspired processing. The focus of all three IRGs is on fundamental understanding, and the knowledge generated along with the tools that are developed are expected to be applicable across a wide variety of problems and challenges, potentially having an impact that can greatly outlast the duration of the IRG.

Besides IRG research, there have been three active years of running Seed competitions, and two Seed projects are currently in operation. The first set of Seeds that were awarded in early 2018 on the broad NSF Big Idea of Quantum Leap and have now concluded with all of the investigators in the three Seeds, now an integral part of the Q-Amase-i NSF Quantum Foundry at UC Santa Barbara. A second round of Seed support was started in 2019 and is reported here: **Selecting for Phase-Separating Nucleic Acid Coacervates**, and **Electronic Structure and Scattering Mechanisms in Twisted Bilayer Graphene**. Separately, UC Santa Barbara successfully competed in the 2018 iSuperSeed2 competition, addressing the Rules of Life Big Idea, with the title, **iSuperSeed: Shape from Activity-Driven Folding: A Path to Materials Morphogenesis**, that kicked off in Fall 2018. An iSuperSeed2 was also jointly awarded to the MRSECs at CU Boulder and UC Santa Barbara on the topic of: **iSuperSeed2: Pathways to the Workforce 2019, a Workshop in Leadership, Communication, and Professional Competencies**. A third Seed award round was competed in 2021, and two new seed projects started, that are reported here, on the topics of

Understanding Thermal Effects on the Microstructure of Additive-Manufactured Materials and Stereochemically Well-Defined Polymeric Materials via Biocatalytic Polymerization.

The Seeds serve the essential role of expanding MRSEC research directions, and perhaps as importantly, bringing in new (and almost always, early-career) investigators. By design, none of the Seed or iSuperSeed investigators have prior IRG involvement. The IRGs as well are not static and believe in continuous process of renewal through the potential addition of new investigators and the occasional transferring out of investigators as well. All three IRGs have added early-career faculty investigators in these past years.

Relationship with the NSF's 10 Big Ideas: While the three IRGs were not explicitly planned around the NSF's 10 Big Ideas, the research is closely allied with at least three of the Big Ideas: **Growing Convergence Research**, for example in the manner in which metallurgists and physicists come together in IRG-1 to develop the next generation of magnetics, and the manner in which biologists and materials scientists come together in IRG-3 to develop the next generation of resilient materials. **Harnessing the Data Revolution** in the manner in which data-driven methods are being employed for imaging in IRG-1 and IRG-3, and the use of machine learning to delve deeper into functional interfaces in IRG-1 and ion transport in IRG-2. **Mid-scale Research Infrastructure** will hopefully be an outcome of IRG-3 as high-throughput rheometry is being developed into a user facility. In contrast to the IRGs, the Seeds were explicitly designed around the Big Questions, and all of the Seeds are either in the area of Quantum Leap or Understanding the Rules of Life (including one of the iSuperSeed2 awards). Finally, the collaborative iSuperSeed2 with CU Boulder mentioned previously falls under the umbrella of **NSF INCLUDES**.

Education and Outreach: UC Santa Barbara MRSEC scientists and education staff are dedicated to improving access to science for a range of different groups, and to building a dynamic workforce of scientists and engineers, and several of the activities have successfully been run remotely during the COVID-19 pandemic. UC Santa Barbara MRSEC education programs provide undergraduate research opportunities, graduate student and postdoctoral mentoring, transferable professional skill training, outreach to K-12 students and teachers, and community outreach. The core MRSEC education/outreach programs are strongly leveraged through other sources of funding allowing, for example, a multiplier effect in the numbers of undergraduate interns that are hosted under the MRSEC umbrella. Thoughtful evaluation of the programs helps monitor progress and ensures agility. Broadening participation of all stakeholders of the UC Santa Barbara MRSEC has the highest priority. Specific attention is paid to increasing the intake and retention of URM students at the graduate and postdoctoral levels. In the past year, there has been a return to in-person outreach activities and in-person internships, which is a welcome change after nearly two years of remote/virtual activities due to COVID-19.

Shared Experimental Facilities: The UC Santa Barbara MRSEC runs world-class shared experimental facilities which sustain and strengthen the impact of the MRSEC and related materials research within UC Santa Barbara, provide for future economic growth through industrial access, enhance workforce training for students and postdoctoral researchers, and provide models for effective functioning and partnerships across the United States. The vision of the SEFs is to sustain the strong community of central, open-access laboratories housing state-of-the-art instrumentation, operated by staff dedicated to user training, support, and collaboration. All equipment in the SEFs is managed by the MRSEC and is available to all members of UC Santa Barbara and surrounding academic/industrial communities. In addition, the UC Santa Barbara leadership continues to lead the growth of the Materials Research Facilities Network (MRFN).

Interaction with Industry: The UC Santa Barbara MRSEC is committed to creating intellectual networks and infrastructure that can benefit workforce preparedness of our students, job creation, industry, and

society. Key industry partnerships include the UC Santa Barbara-Mitsubishi Chemical Center for Advanced Materials. Established in 2001, it is led by **Fredrickson** who also coordinates all UC Santa Barbara MRSEC Industrial Outreach. The Dow Materials Institute at UC Santa Barbara (started 2011, led by **Hawker**) works with the UC Santa Barbara MRSEC in a number of synergistic ways. Both are co-located with the UC Santa Barbara MRSEC. Examples of the synergies include support for facilities, co-staffing with the MRSEC leading to efficiencies, the provision of graduate fellowships, travel grants, and support to the Graduate Students for Diversity in Science organization. A third recent emerging partnership has been with the chemical giant BASF, through the California Research Alliance (CARA) that has been supporting a growing number of UCSB MRSEC researchers as well. Annually, industrial partners meet with UC Santa Barbara MRSEC faculty, graduate students, and postdoctoral researchers at a two-day symposium, the Materials Research Outreach Program (MROP), which was held in January 2022, virtually. This event also usually involves PREM partners, and talks appropriate for a general audience are specially advertised, illustrating the integration of stakeholders at all levels.

Center Management: There have been some significant changes in the management structure of the UC Santa Barbara MRSEC in recent years. The new Co-PI and Associate Director, **Bates**, took the reins from **Jayich** who now co-Directs the Q-Amase-i NSF Quantum Foundry at UC Santa Barbara. The PI and Co-PI report to the Dean of Engineering at UC Santa Barbara. The Dean, in turn, works in close consultation with the Dean of Mathematics, Life, and Physical Sciences and the Vice Chancellor for Research to ensure the success of the MRSEC. **Hawker** serves as the coordinator of the SEFs, and **Fredrickson** and **Pak** are the other senior investigators who comprise the overall leadership team, with various responsibilities. Other changes in the leadership include **Read de Alaniz** replaced by **Pitenis** as the Diversity Officer, and **Shea** replaced by **Clément** in leading International Activities. The Executive Committee is an internal body comprising IRG Co-Leaders and all of the above individuals. The External Advisory Board (EAB) comprises eight members: Professors Nitash Balsara (UC Berkeley/LBNL), Dan Frisbie (Minnesota), Heather Maynard (UCLA), Stuart Rowan (Chicago), Pat Woodward (Ohio State), and Dr. Michelle Johannes (Naval Research Lab). All other members started in late 2015, and continue to play an active role, for example, in the Seeds competition. Prof. Luis Echegoyen, the founding director of the PREM at UT El Paso has been retained from the previous board. Professor Ka Yee Lee has stepped down from the EAB, as she took the role of Provost at the University of Chicago.

1B. Center Accomplishments for Current Reporting Period

INTELLECTUAL MERIT

The research accomplishments of the three IRGs are summarized below. Numerous collaborative publications that acknowledge this grant have appeared in the literature, with statistics presented in the appendix. The first three Seeds projects that started in 2018 have completed and are not reported here. Two projects from 2019, and two from 2021 are summarized, as are the iSuperSeed2 projects that resulted after a MRSEC-wide competition in late 2018.

IRG-1: Magnetic Intermetallic Mesostructures focuses on structure-property relationships in intermetallics and the interrelationships between magnetism, strain, temperature, and chemistry. Previous work arising from this project has built both a theoretical, modeling, and experimental framework to predict and measure magnetic ground states and to control their local magnetic responses via engineered elastic strain fields owing to external forces or microstructurally-induced fields. Major advances during this reporting period include the development of a comprehensive first-principles study and materials design framework for identifying optimal alloying additions in tetragonal Heusler materials to reside on

or near phase boundaries of spin spiral states. These predictions are of particular interest as the marginal stability of these designed alloys should render them susceptible to small perturbations, thereby providing experimental guidance for materials that show strong coupling between magnetism and mechanical strain. Notable other advances include a multiscale investigation of additively manufactured metallic magnetic materials using 3D tomography techniques and detailed electron microscopy. These advanced characterization approaches demonstrated the link between printing-induced porosity and degradation of magnetic properties, as well as the development of spinodal decomposition within the grain interiors. A prevailing theme in IRG research is a tightly integrated feedback loop between experimental and computational efforts that drives new science.

IRG-2: Polymeric Ionic Liquids (PILs) focuses on developing the design rules to translate the properties of ionic liquids onto solid supporting polymers. This includes the development of synthetic routes necessary to build PIL-based functional and adaptive materials capable of high ionic conductivity, high ion selectivity, light-responsive behavior, and redox-activated ion/electron-mixed conduction. In this reporting period, IRG-2 researchers and collaborators have studied the chain conformation of PILs by small-angle neutron scattering and constructed the phase diagram of PIL complexes with equilibrium self-consistent field theory, suggesting a promising route to compatibilize immiscible polymer blends. Moreover, researchers demonstrated that tethering bulky zwitterions to the side chains of a polymer results in a semi-crystalline morphology with exceptionally high lithium conductivity that decouples ion motion from polymer segmental motion. Researchers also observed high proton conductivity in a PIL block copolymer that forms a lamellar microphase structure, the high conductivity achieved through Grothuss proton hopping coupled with reduced polymer segmental motion. These insights have revealed an entirely new set of design rules for high-performance solid polymer electrolytes. Further synthetic advances enabled optimization of high-performance PIL-based polymers with selective ligands and graft densities, and also allowed for photoresponsive PILs used as multiwavelength photodetectors.

IRG-3: Resilient Multiphase Soft Materials aims to understand and develop new syntheses, processing schemes and structure-property relationships for ultrastrong, ultratough soft materials by understanding and capturing the processing and features of materials produced by marine organisms. Through careful analysis of some of the toughest and hardest known organic and composite natural materials, including the mussel byssus, squid beak and bloodworm jaw, we seek to understand how nature utilizes non-equilibrium assembly and phase transformation processes to synthesize multi-phase materials with carefully controlled morphologies, interphases and interfaces across a hierarchy of length scales, while at the same time investigating how such structuring achieves superior mechanical performance. We then aim to translate these features to the development of new synthetic materials and processing methods. Research in IRG-3 during the current reporting period falls along three broad themes: (i) bioinspired chemistries for functional materials, (ii) understanding and controlling non-equilibrium processing, and (iii) mechanics of architected bio-inspired materials. Major advances during this reporting period include: elucidating the separate roles of chain topology and block architecture in controlling interactions that lead to polymer assembly of acrylate-based polymers; the discovery that competing interactions in mixtures of intrinsically disordered proteins and nucleic acids produce multi-phase coacervates; identifying the role of cation- π interactions in peptide adhesive performance; the integration these findings to create biomimetic polymeric ionic liquids with versatile adhesive properties; the discovery of nanolattice architectures in the swell shark egg case and its role in achieving high toughness, and the design of new 3D printing modalities for emulating them in elastomeric foams and composites.

Seeds and iSuperSeed2: In 2019, two new Seeds were awarded to two teams of two faculty members each, who had no prior experience of collaborating. Reports from these are attached, and they appear to be

headed in promising directions. These are on the subjects of **Selecting for Phase-Separating Nucleic Acid Coacervates**, and **Electronic Structure and Scattering Mechanisms in Twisted Bilayer Graphene**. Separately, after internal campus screening, two proposals went to the NSF for the iSuperSeed2 competition and one was successful, addressing the Rules of Life Big Idea, with the title **iSuperSeed2: Shape from Activity-Driven Folding: A Path to Materials Morphogenesis**, that kicked off in Fall 2018. This iSuperSeed2 is impacting the culture of the UC Santa Barbara campus around areas at the interface of active matter and living cells and their development. A second **iSuperseed2: Pathways to the Workforce 2020: A Workshop in Leadership, Communication, and Professional Competencies** was awarded jointly to MRSEC Education Directors **Pak** at UC Santa Barbara and Christine Morrow at CU Boulder to develop a workshop to address the NSF INCLUDES Big Idea around developing STEM talent from all sectors of society. In 2021, we ran a final Seed competition, and two seed grants were awarded to Assistant Professor **Yanying Zhu (Understanding Thermal Effects on the Microstructure of Additive-Manufactured Materials)** and Assistant Professor **Yang Yang (Stereochemically Well-Defined Polymeric Materials via Biocatalytic Polymerization)**.

This has been a good year for awards and honors to MRSEC Faculty and students. A select sampling is presented here. During this reporting period **Bates** was awarded a Camille Dreyfus Teacher-Scholar Award and an *ACS Polymers Au* Rising Star in Polymers Award. **Clément, Pitenis, and Yang** were all awarded the National Science Foundation Career Award. **Liao** has won Early Career Awards from, NASA, AFOSR, and ONR. This was also the year when **Fredrickson** was elected Member, National Academy of Sciences, and **Van der Ven** was awarded the TMS William Hume-Rothery Award. Among our students, Marcela Areyano and George Degen were awarded University Awards of Distinction. George Degen was also selected to attend the 2021 Lindau Nobel Laureate Interdisciplinary Meeting as a University of California Delegate. Patrick Getty was awarded an NSF Graduate Research Fellowship.

BROADER IMPACTS

Shared Facilities, comprising experimental facilities and high-performance computing facilities, are central to UC Santa Barbara MRSEC research, and play a key role in serving collaborators, industrial partners, and local start-up companies. All of the UC Santa Barbara facilities are utilized by multiple companies that are current members or alumni of the New Venture Competition and the Technology Management Program, both of which are partners of the MRSEC Industrial Outreach. Several of those companies were founded by former MRSEC students who benefited from the MRSEC Shared Facilities, and as they plan their evolution, the continued use of the facilities plays a role in their thinking.

Education and Outreach is an important pillar of UC Santa Barbara MRSEC engagement, and ranges in impact from K–12, school teachers and the general public, all the way through mentoring undergraduate and graduate students, and postdoctoral fellows. Despite the several challenges associated with the COVID-19 pandemic, several of the activities continued apace, including remote internships and activities for K–12 students and presentations to the public over the Zoom platform. We are increasingly returning to in-person K-12 activities and a full range of in-person summer internships, including our international exchanges.

2. LIST OF CENTER PARTICIPANTS

i. Primary Participant (PP):

Christopher Bates	Asst. Professor	Materials	Co-PI and Assoc. Director, IRG-2
Mark Bowick	Deputy Director	Kavli Institute for Theoretical Physics	iSuperSeed
Michael Chabinyo	Professor	Materials	IRG-2
Bradley Chmelka	Professor	Chemical Engineering	IRG-3
Raphaële Clément	Asst. Professor	Materials	IRG-2, International Programs
Samantha Daly	Professor	Mechanical Engineering	IRG-1
Zvonimir Dogic	Professor	Physics	iSuperSeed
Glenn Fredrickson	Professor	Chemical Engineering	IRG-2, IRG-3, Industry
Daniel Gianola	Professor	Materials	IRG-1
Craig Hawker	Professor	Materials, Chemistry & Biochemistry	IRG-2, IRG-3, Facilities
Matthew Helgeson	Assoc. Professor	Chemical Engineering	IRG-3
Ania Jayich	Professor	Physics	Co-PI, IRG-1
Bolin Liao	Asst. Professor	Mechanical Engineering	IRG-1
M. Cristina Marchetti	Professor	Physics	iSuperSeed
Robert McMeeking	Professor	Mechanical Engineering, Materials	IRG-3
Thuc-Quyen Nguyen	Professor	Chemistry & Biochemistry	IRG-2
Dorothy Pak	Academic Coordinator III	Materials Research Laboratory, MSI	Education Director
Angela Pitenis	Asst. Professor	Materials	IRG-3, Diversity Coordinator
Tresa Pollock	Professor	Materials	IRG-1
Javier Read de Alaniz	Professor	Chemistry & Biochemistry	IRG-2
Omar Saleh	Professor	Materials, BMSE	Seed
Rachel Segalman	Professor	Chemical Engineering	IRG-2
Ram Seshadri	Professor	Materials, Chemistry & Biochemistry	PI and Director, IRG-1
Joan-Emma Shea	Professor	Chemistry & Biochemistry, Physics	IRG-3
Sebastian Streichan	Asst. Professor	Physics	iSuperSeed
Megan Valentine	Professor	Mechanical Engineering	IRG-3
Anton Van der Ven	Professor	Materials	IRG-1
Vojtech Vlcek	Asst. Professor	Chemistry & Biochemistry	Seed
Herbert Waite	Professor	MCDB, Chemistry & Biochemistry	IRG-3
Stephen Wilson	Professor	Materials	IRG-1
Yang Yang	Asst. Professor	Chemistry	Seed
Andrea Young	Assoc. Professor	Physics	Seed
Yangying Zhu	Asst. Professor	Mechanical Engineering	Seed

Bold: IRG Co-Leader

ii. Primary National Labs and/or International Participants (PNIP)

None

iii. Secondary Participants (SP)

None

iv. Affiliated Participants (AP):

Leon Balents	Professor	Physics, KITP, UCSB
Szabolcs Berezvai	Assistant Professor	Budapest University of Technology, Hungary
Irene Beyerlein	Professor	Mechanical Engineering, UCSB
Jamie Booth	Professor	California State University, Northridge
Irene Chen	Professor	UC Los Angeles
Noy Cohen	Assistant Professor	Technion Institute of Technology, Israel
Marc de Graef	Professor	Carnegie Mellon University
Claus Eisenbach	Professor	University of Stuttgart, Germany
Amalie Frischknecht	Scientist	Sandia National Laboratory
Songji Han	Professor	Chemistry & Biochemistry, Chemical Engineering, UCSB
Attila Kossa	Associate Professor	Budapest University of Technology, Hungary
Olivier Thomas	Professor	Aix-Marseille University, France

Abbreviations:

MSI = Marine Science Institute

BMSE = Biomolecular Science and Engineering

MCDB = Molecular, Cellular, and Developmental Biology

v. Users of Shared Facilities (USF)

Alison Butler / Chemistry and Biochemistry

Andrea Young / Physics

Angela Pitenis / Materials Department

Ania Jayich / Physics

Arnab Mukherjee / Chemical Engineering

Ben Mazin / Physics Department

Bolin Liao / Mechanical Engineering

Bradley Chmelka / Chemical Engineering

Brandon Greene / Chemistry and Biochemistry

Carlos Levi / Materials Department

Carolynn Culver / Marine Sciences Institute

Chris Bates / Materials Department

Christopher Hayes / Molecular, Cellular and Developmental Biology

Christopher Palmstrom / Materials Department

Craig Hawker / Materials Department

Cyrus Safinya / Materials Department

Dan Gianola / Materials Department

Daniel Morse / Institute for Collaborative Biosciences

Debora Iglesias-Rodriguez / Ecology, Evolution, and Marine Biology

Douglas Kennett / Anthropology

Elliot Hawkes / Mechanical Engineering

Eric McFarland / Chemical Engineering

Frank Zok / Materials Department

Frederick Dalhquist / Chemistry and Biochemistry

Gabriel Menard / Chemistry and Biochemistry

Galan Moody / Electrical and Computer Engineering

Galen Stucky / Chemistry and Biochemistry
Guillermo Bazan / Chemistry and Biochemistry
Herbert Waite / Molecular, Cellular and Developmental Biology
Javier Read de Alaniz / Chemistry and Biochemistry
Jim Speck / Materials Department
John Bowers / Electrical and Computer Engineering
Jonathan Klamkin / Electrical and Computer Engineering
Karen Szumlinski / Psychology
Kenneth Kossik / Molecular, Cellular and Developmental Biology
Kevin Plaxco / Chemistry Department
Kunal Mukherjee / Materials Department
Lior Sepunaru / Center of Polymers and Organic Solids
Mahdi Abu-Omar / Chemistry and Biochemistry
Mark Rodwell / Electrical and Computer Engineering
Mark Sherwin / Physics
Mattanjah De Vries / Chemistry and Biochemistry
Matthew Begley / Engineering
Matthew Fisher / Physics
Matthew Helgeson / Chemical Engineering
Megan Valentine / Mechanical Engineering
Michael Chabynec / Materials Department
Michael Gordon / Chemical Engineering
Michelle O'Malley / Chemical Engineering
Norbert Reich / Chemistry and Biochemistry
Omar Saleh / Materials Department
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Phil Christopher / Chemical Engineering
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Rachel Segalman / Chemical Engineering
Ram Seshadri / Materials Department
Raphael Clement / Materials Department
Ryan Stowers / Mechanical Engineering
Sarah McClure / Anthropology
Shuji Nakamura / Materials Department
Songi Han / Chemistry and Biochemistry
Sriram Krishnamoorthy / Materials Department
Stephen Wilson / Materials Department
Steve Buratto / Chemistry and Biochemistry
Steven Denbaars / Materials Department
Sumita Pennathur / Mechanical Engineering
Susannah Scott / Chemical Engineering
Susanne Stemmer / Materials Department
Thomas Weimbs / Molecular, Cellular and Developmental Biology
Tresa Pollock / Materials Department
Trevor Hayton / Chemistry and Biochemistry
Umesh Mishra / Electrical and Computer Engineering
Yangying Zhu / Mechanical Engineering
Zvonimir Dogic / Physics

3. LIST OF CENTER COLLABORATORS

Collaborator	Institution	e-mail	Expertise	IRG/ Seed	Shared Facility User
Athina Anastasaki	ETH Zurich, Switzerland	athina.anastasaki@mat.ethz.ch	Polymer Synthesis	IRG-2, IRG-3	No
Shane Ardo	University of California, Irvine	ardo@uci.edu	Drug Delivery		Yes
Rob Atkin	University of Western Australia	Rob.Atkin@uwa.edu.au	Polymer Chemistry	IRG-2	No
Cyrille Boyer	University of New South Wales, Australia	cboyer@unsw.edu.au	Polymer Synthesis	IRG-2, IRG-3	No
Michele Ciavarella	Polytechnic University of Bari, Italy	michele.ciavarella@poliba.it	Fracture of polymers and viscoelastic solids	IRG-3	No
Jingyi Chen	University of Arkansas	chenj@uark.edu	Hybrid Materials		yes
Daniel Cotton	Monterey Institute for Research in Astronomy	dc@mira.org	Optical Components		Yes
Carolyn Culver	Marine Sciences Institute	c_culver@lifesci.ucsb.edu	Marine Toxins		Yes
Vikram Deshpande	Cambridge University, UK	vsd20@cam.ac.uk	Biomaterials and Biomechanics	IRG-3	No
Bruce Dunn	University of California, Los Angeles	bdunn@ucla.edu	Battery Materials		Yes
Lyndon Emsley	Ecole Polytechnique Federal de Lausanne, (EPFL) Switzerland	lyndon.emsley@epfl.ch	NMR Spectroscopy	IRG-3	No
Mark Field	Rigetti & Co. Inc.	mark.field@rigetti.com	Magnetic Properties of Films		Yes
Benny Freeman	University of Texas, Austin	freeman@che.utexas.edu	Membrane Science	IRG-2	No
Fumihiko Shimizu	Mitsubishi Chemical Corporation	shimizu.fumihiko.mu@m-chemical.co.jp	Polymer Films	IRG-3	No
Sukriti Gakhar	Ascendis Pharma	sgr@ascendispharma.com	Medical		Yes
Stephan Hecht	Humboldt University of Berlin, Germany	sh@chemie.hu-berlin.de	Photochemistry	IRG-2	No
Thomas Holzheu	Chemistry of Concrete, LLC	tholzheu@concrete-lab.com	XRF		Yes

MATERIALS RESEARCH SCIENCE AND ENGINEERING CENTER AT UC SANTA BARBARA

Songong Hwang	California Institute of Technology	sonjong@cheme.caltech.edu	Catalysis		Yes
Eiko Ino	Asahi Kasei Corp	eiko_ino@ucsb.edu	Polymer Chemistry	IRG-2	Yes
Timothy James	Bioprotonics LLC	t.james@bioprotonics.com	MRI		Yes
Ryan Jansonius	Ionomr Innovations	rjansonius@ionomr.com	Thermal degradation of synthetic fabrics		Yes
Mercouri Kanatzidis	Northwestern University	m-kanatzidis@northwestern.edu	Hybrid Halides	IRG-1	Yes
Bumjoon Kim	KAIST, South Korea	bumjoonkim@kaist.ac.kr	Polymer Physics	IRG-3	No
Karen Krawczyk	MSI Transducer	kkrawczyk@msitransducers.com	Manufacturing contamination		Yes
Kevin S. Kung	Takachar LTD	kevin@takachar.com	Biomass Feedstock Materials		Yes
David Laitar	Dow Chemical	DLaitar@dow.com	Polymer Synthesis	IRG-3	No
Chris Leighton	University of Minnesota	leighton@umn.edu	Neutron Scattering	IRG-1	No
Li Li	Braskem Petrochemical	li.li@braskem.com	Catalysis		Yes
Feng Lin	Virginia Tech	fenglin@vt.edu	Energy Storage		Yes
Nate Lynd	University of Texas, Austin	lynd@che.utexas.edu	Polymer Chemistry	IRG-2	No
Cheng-Kang Mai	Phenomenex Inc	ChengKangM@phenomenex.com	Inorganic Materials		Yes
Lucymarie Mantese	Mojo Vision	lucymarie.mantese@mojo.vision	PLQY of quantum dots		Yes
Kris Mayjaszewski	Carnegie Mellon	km3b@andrew.cmu.edu	Polymer Synthesis	IRG-2, IRG-3	No
Daniel McKeown	Becker Studios Construction	daniel@beckercon.com	Building Materials		Yes
Bert Meijer	Eindhoven University of Technology, Netherlands	e.w.meijer@tue.nl	Polymer Synthesis	IRG-3	No
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Robert Miller	Marine Sciences Institute	rjmiller@ucsb.edu	Marine Toxins		Yes
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MATERIALS RESEARCH SCIENCE AND ENGINEERING CENTER AT UC SANTA BARBARA

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Michael Persson	Chalmers University of Technology, Sweden	michael.persson@chalmers.se	Silica Chemistry	IRG-3	No
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MATERIALS RESEARCH SCIENCE AND ENGINEERING CENTER AT UC SANTA BARBARA

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4. STRATEGIC PLAN

The Strategic Plan for the UC Santa Barbara MRSEC has been evolving given that we are nearing the last year of the project, and wish to take stock of what the next year holds in terms of the MRSEC competition. We have spent much of this past year recovering from the impacts of COVID-19, and in many aspects we believed we have fully recovered, for example, the full and robust functioning of labs and facilities. The effects of having graduated several cohorts of students and postdoctoral fellows is still being felt, with slowed on-boarding of new researchers and in executing new projects. Nevertheless, this is an exciting time and we are optimistic, particularly in light of productivity as measured by several metrics, for example, a return to in-person K–12 outreach activities and undergraduate internships having almost been restored to pre-COVID-19 levels.

The goals and desired outcomes of the MRSEC are described below, with quantifiable actions (which also serve as metrics) for the various components of the MRSEC.

Research (IRGs)	
Goal: Fostering a collaborative, interdisciplinary research culture, and creating lasting value	Strategy: Increase proportion of multi-PI publications through shared advising; initiate new collaborations across domains; integrate experiment and theory; advance methods and techniques that have lasting utility.
Research (Seeds)	
Goal: Pursuing new directions, and involving new investigators	Strategy: Involve new investigators in the MRSEC; evolve current IRG research in new directions; and/or seed the creation of new IRGs. No more new Seed funding is planned, and the successful outcomes of all awarded seeds has been presented in the summary.
Facilities (SEF)	
Goals: Enabling world-class research and development for UC Santa Barbara, and for local industry; support efforts nationwide	Strategy: Increase the number of SEF users through better publicity; increase the proportion of off-campus users; add new capabilities; and maintain fiscal sustainability; provide professional development opportunities for SEF technical staff.
Undergraduate Education	
Goals: Developing a highly trained and diverse future STEM workforce	Strategy: Initiate start-up internship program; continue mentoring of diverse cohorts of school-year and summer interns, encourage a high percentage to pursue grad school and other STEM careers.
Graduate education	
Goal: Training for a collaborative and inclusive culture of creative research	Strategy: Increase the percentage of MRSEC graduate students co-advised by two or more MRSEC senior investigators; support Graduate Students for Diversity in Science to expand horizons.
K–12 Teachers	
Goal: Supporting K–12 educators to incorporate materials research into curricula	Strategy: Help teachers to create new curricular content that incorporates recent advances in materials and supports the Next Generation Science Standards.
General public	
Goal: Engaging the public with exciting new advances in materials research	Strategy: Collaborate with the Wolf Museum of Exploration and Innovation (MOXI). Expand the pilot of Art+Energy program for K-12 students, events for the public.

5 RESEARCH ACCOMPLISHMENTS AND PLANS

IRG-1: Magnetic Intermetallic Mesostructures

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Overview: The materials challenge addressed in this IRG is to understand and develop unprecedented control over the couplings between strain, magnetization, and temperature (entropy) in single- and multiphase intermetallic compounds. The goals of the IRG are to: (i) elucidate emergent magnetic phenomena in strain and composition gradients, where local symmetry breaking through engineered biphasic systems or externally imposed lattice strain fields will allow for novel phenomena that are absent in the homogeneous phase, (ii) develop new helical magnets and manipulate chemical and crystallographic features to control complex ordered states (*e.g.* skyrmion lattices) that may yield novel magnetocalorics, and (iii) identify and understand atomistic, crystallographic and nano/microstructural mechanisms of magnetic actuation mediated by spin frustration. The long-term outcome of this research will be design rules for novel intermetallics that display engineered magnetoelastic and magnetocaloric responses to external fields, which will provide a fundamental advance capable of impacting technologies of actuation and solid-state refrigeration.

Research Progress:

Tuning magnetic antiskyrmion stability in tetragonal inverse Heusler alloys. A variety of applications, including spintronics, require magnetic materials that can host exotic spin textures at room temperature, such as skyrmion and antiskyrmion phases. While it is common to alter the relative stability of different magnetic phases by varying temperature and magnetic field, there is also a desire to identify materials whose magnetic phases can be controlled and modified with electric fields and/or mechanical perturbations. The magnetic properties of a material are most sensitive to changes of external boundary conditions when the material is close to a magnetic phase transition. One approach to creating materials whose magnetic properties can easily be manipulated is to implement alloying strategies that push promising magnetic materials closer to magnetic phase boundaries. This makes it likely that small perturbations, such as strain, can induce magnetic transitions. IRG-1 researchers performed a comprehensive first-principles study of the effects of alloying on magnetic materials in order to identify

chemical compositions that are close to phase boundaries of spin-textured magnetic phases [1]. The focus was on tetragonal inverse Heusler phases (**Fig. 1a**) with chemical formula Mn_2XY where X corresponds to late transition metals and where $Y=Ga, Sn, In$. The tetragonal symmetry of this class of compounds arises from a martensitic transformation. The symmetry is sufficiently low to allow for the formation of topological spin textured phases, such as skyrmions and antiskyrmions, that can be stable up to the Curie temperature, which is often above room temperature in these materials. The inverse Heusler phases are very amenable to alloying, especially on the X sublattice, with variations of transition metal composition potentially altering their magnetic interactions between the different sublattices of the inverse Heusler

compound (**Fig. 1b**). A systematic computational and theoretical study was performed to identify alloy compositions within the inverse Heusler crystal structure that are at the edge of phase boundaries between different spin spiral phases. The general computational approach is schematically illustrated in Figure 1 and involved analyses at several length scales. As a first step, the magnetic properties of inverse Heusler phases were investigated parametrically at the atomic and meso scales using a generalized Heisenberg magnetic Hamiltonian and coarse-grained free energy models. The objective was to map out the type of magnetic phases that can be supported by the tetragonal inverse Heusler crystal structure as a function of magnetic interaction parameters (i.e., the exchange, Dzyaloshinskii-Moriya coupling terms and anisotropy coupling terms). Magnetic phase diagrams were then constructed as a function of the magnetic coupling interaction parameters. Since the chemistry of a particular compound determines the strength of the magnetic interactions, each compound corresponds to a point in these phase diagrams (e.g. points A and B in the coarse-grained phase diagram of **Fig. 1c**). First-principles electronic structure calculations were then performed on a large number of promising inverse-Heusler compounds to determine their magnetic interactions and thereby identify where each compound lies in the magnetic phase diagrams in terms of magnetic interactions. This made it possible to identify pairs of compounds (e.g. Mn_2AY and Mn_2BY) that reside on opposite ends of phase transition lines, which then become the natural end members of alloyed inverse Heusler phases (i.e., $Mn_2A_{1-z}B_zY$).

The properties of promising pseudo-binary alloys were next investigated in more detail from first-principles. **Fig. 2a**, for example, shows the variation of the magnetic anisotropy interaction term K as a function of composition z for three pseudo-binary inverse Heusler $Mn_2Pt_{1-z}X_zGa$ ($X=Au, Ni, Ir$) using three different approaches to model disordered solid solutions. The variation of the magnetic interactions as a function of composition for the three pseudo-binaries are shown in **Fig. 2b**. As is clearly revealed in **Fig. 2b**, all three pseudo-binaries cross a variety of magnetic phase boundaries involving spin-textured phases, making these alloys promising materials for actuating applications, where small perturbations such as strain will trigger large changes in magnetic properties. A final step was to analyze the stability of the

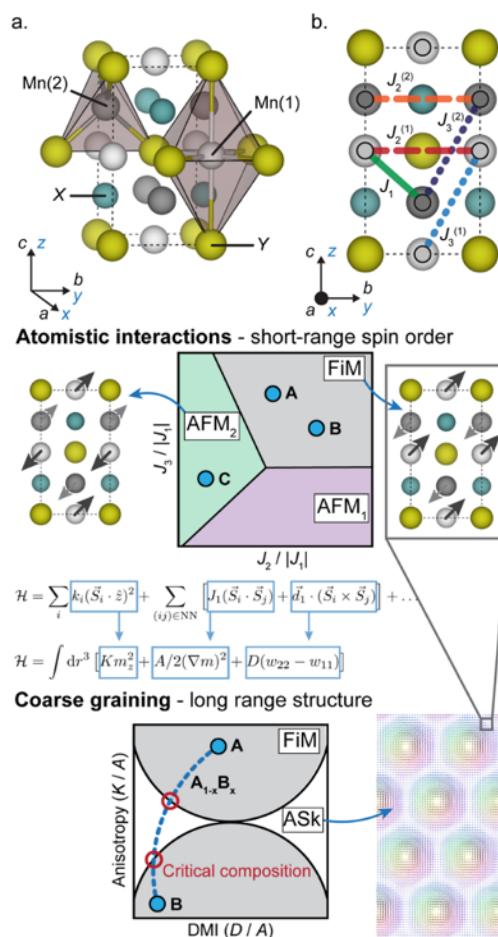


Fig. 1. (a) The tetragonal inverse Heusler crystal structure; (b) The magnetic interactions of the atomic Heisenberg model; (c) The multi-scale computational approach to identify promising alloys.

pseudo-binary inverse Heusler alloys to determine if and under which conditions their solid solutions are stable. **Fig. 2c**, for example, shows the calculated mixing energy and corresponding phase diagram for the three promising pseudo-binary inverse Heusler alloys. Other calculations of phase stability were also performed to assess under what conditions promising alloy compositions can be synthesized. These computational predictions have informed experimental efforts within the IRG that are directed at synthesizing alloyed inverse Heusler compounds whose magnetic properties can be manipulated by strain.

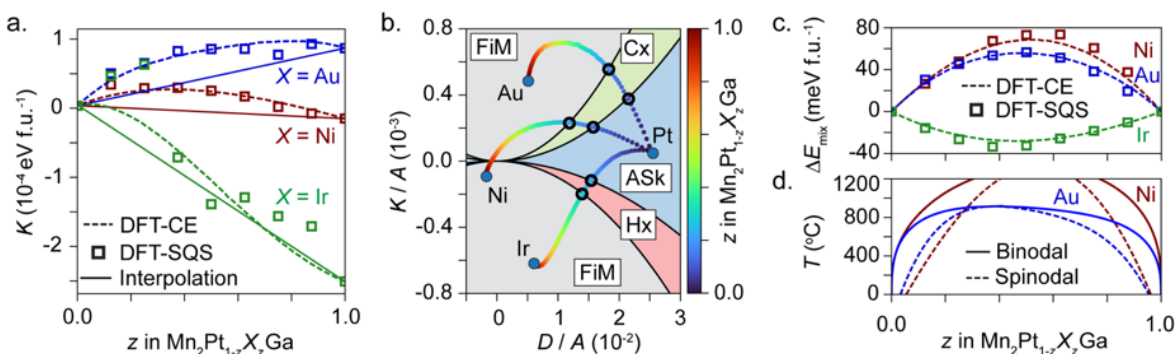


Fig. 2. (a) The variation of the anisotropy interaction term of the coarse-grained magnetic free energy as a function of alloy composition in $\text{Mn}_2\text{Pt}_{1-z}\text{X}_z\text{Ga}$, with $X=\text{Au}, \text{Ni}, \text{Ir}$, as calculated with three different approaches. (b) The phase diagram of the coarse-grained free energy as a function of its materials parameters (A =exchange coefficient, D =Dzyaloshinskii-Moriya coefficient and K =anisotropy interaction) and the paths of the pseudo-binary $\text{Mn}_2\text{Pt}_{1-z}\text{X}_z\text{Ga}$, with $X=\text{Au}, \text{Ni}, \text{Ir}$ alloys in this phase diagram. (c) Calculated energy of mixing and binodal and spinodals for the three pseudo-binary alloys.

Microstructural evolution in additively manufactured magnetic materials. Additive manufacturing (AM) is becoming widely used for manufacturing due to the reduction in total number of components in a system and the ability to realize complex design geometries previously inaccessible. The direct printing of functional materials is not as widely explored yet, with the ability to build permanent magnets into complex geometries for use in actuators and electric motors being particularly attractive for increasing performance and reducing weight. Alnico permanent magnets (Al-Ni-Co-Ti-Cu-Fe alloy) have been shown to possess relatively temperature-independent magnetic properties up to 400 °C, which has facilitated the use of Alnico magnets in traction motors and generators.

Alnico alloys are chemically similar to Ni- and Fe- alloys that are already amenable to AM processes, allowing for the fabrication of near-net shape parts that would further broaden the application space. Since Alnico material is hard to mechanically work into final shapes, any near net shape manufacturing is a major advantage. This is especially relevant for small magnets, for example those integrated into electrical switches, speakers, or buried magnets for motor applications.

The arrangement of phases and the microstructure of Alnico strongly influences its magnetic properties. IRG-1 researchers printed samples of Alnico by selective laser melting (SLM), for the first time [4], and their microstructure investigated in 3D at the mm^3 -scale using the femtosecond-laser enabled TriBeam microscope (**Fig. 3**). This 3D data revealed large pores with a mean

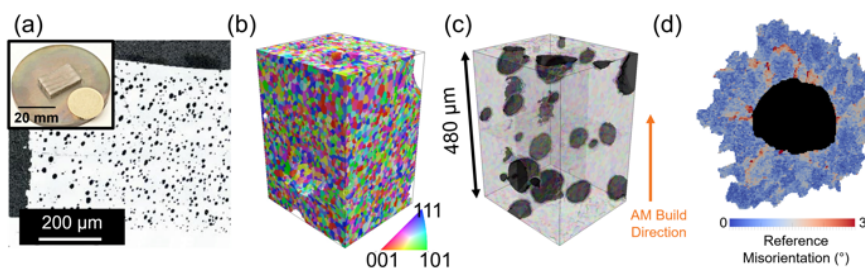


Fig. 3. Alnico magnets were printed in (a) and the 3D grain orientations were mapped (b) in relation to the distribution of pores (c). Large orientation gradients are observed surrounding the pores, both of which will be mitigated through future print parameter optimization.

diameter of 42 μm and spherical shapes, these pores are likely due to gas porosity in the initial powder feedstock and gas entrapment during the SLM print process. The grain structure is equiaxed with average diameter of 11 μm (similar to powder metallurgy routes), with the grains surrounding the pores containing misorientation gradients of 4-5°. This contrasts with columnar microstructures typical of additively manufactured metals, which can easily have misorientation gradients approach 15–20°. The pores are clearly detrimental to the bulk magnetic properties of the material and have been shown to be mitigated with further print parameter optimization. The grain interiors of the 3D printed part have high volume fractions of the same magnetic spinodal $\alpha_1//\alpha_2$ phase observed in conventionally fabricated Alnico, which gives rise to a coercivity (H_c) of 51.2 kA m^{-1} . The spinodal phase in Fig. 4b is only disturbed near some of the grain boundaries in (a,c) where the high contrast α_γ forms, locally depleting Fe and promoting the formation of α_2 instead of the desired spinodal $\alpha_1//\alpha_2$. Despite the porosity and low volume fractions of α_γ , the additively manufactured Alnico material is promising due to its equiaxed grain structure, high volume fraction of the spinodal and reasonable coercivity value. SLM processing route optimization and subsequent thermos-magnetic heat treatments are likely to, respectively, reduce porosity and suppress the formation of α_γ .

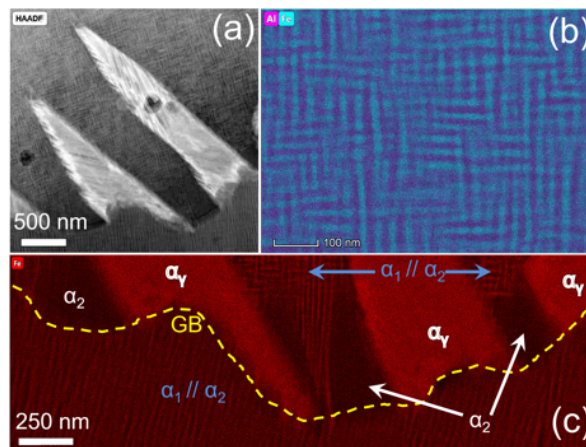


Fig. 4. TEM images of the as-printed Alnico material show the highly coherent fine-scale spinodal $\alpha_1//\alpha_2$ nanostructure (a,b), which give rise to the magnetic properties that are comparable to conventionally processed Alnico. The detrimental α_γ phase is also observed along grain boundaries, which likely could be eliminated with further thermo-magnetic heat treatments.

Future Plans:

Magnetism and mechanics in Heusler alloys. During the current reporting period, IRG-1 researchers predicted that the magnetism of tetragonal inverse Heuslers can be tuned through changes in composition that introduce local strain [1] via density functional theory calculations to identify several likely candidates within this large family of compounds. Recently, IRG-1 researchers have been working to experimentally validate these calculations. Specifically, IRG-1 researchers have prepared a series of Heusler intermetallics with the general formula $\text{Mn}_2\text{Rh}_{1-x}\text{Ir}_x\text{Sn}$ to investigate how local strain from iridium substitution affects the magnetic behavior of the skyrmion host Mn_2RhSn and compare these experimental results to the calculated magnetic phase diagrams. Future work will continue preparing these materials, confirming their quality, and conducting extensive magnetic characterization.

Additional work on this class of materials is motivated by their magnetic interactions that strongly depend on interatomic coupling distances and local chemical order, making plastic deformation an effective mechanism to control magnetism. The Heusler intermetallic MnCu_2Al is particularly well suited to investigate this coupling between magnetism and mechanical deformation, with room-temperature ferromagnetism and which deforms plastically. IRG-1 researchers have recently demonstrated the dramatic decrease of ferromagnetic saturation after plastic deformation of MnCu_2Al by compression or grinding. These experiments indicate a high degree of coupling between magnetism and plastic deformation in this intermetallic alloy, suggesting that the converse relationship may also exist. Through a combination of experimental and computational methods, IRG-1 researchers hope to determine whether the long-range magnetic interactions hosted in MnCu_2Al could be sufficient to alter the deformation energy landscape for dislocations and their motion. The single ordered magnetic sublattice in MnCu_2Al makes it an ideal model

system for isolating the impacts of magnetism on plastic deformation and IRG-1 researchers are using Phase Field Dislocation Dynamics to computationally investigate dislocation motion in MnCu_2Al both with and without magnetic interactions. These results will be compared with a thorough investigation of dislocation nucleation and dynamics in MnCu_2Al *via in-situ* microLaue experiments and subsequent investigation of the deformed region using magnetic TEM.

Understanding phase separation in Heusler compounds. Half-Heusler and Heusler compounds, with chemical formulas XYZ and XY_2Z and crystal structures C1_b and L2_1 , respectively, have been prepared from a wide variety of elements where, in general, the X-site and Y-site correspond to an earlier and later transition metal, and the Z-site is occupied by a main group element. The exceptional properties of these compounds derive from their broadly varying material properties that are readily controlled *via* valence electron count. Despite the innate power of leveraging valence electron count to predict the properties of these materials, the feasibility of capturing the predicted properties through a chemically doped solid solution is often willfully overlooked. IRG-1 researchers are in the process of identifying a simple proxy based on first-principles electronic structure-based modeling that demonstrates phase separation—and conversely, the propensity for solid-solution formation—in half-Heusler and Heusler compounds is strongly linked to the electronic behavior of the end-members. Preliminary findings suggest that alloying between distinct pairs of half-Heusler and Heusler compounds is possible at accessible processing temperatures when the two end-members are isoelectronic. However, the formation of a band gap in semiconducting half-Heusler compounds is associated with significant stabilization. Attempts to create solid solutions with a semiconducting half-Heusler compound therefore leads to phase separation across the tie line because of the energy penalty associated with filling states in the gap. The simple proxy related to the electronic structure developed here will differentiate between Heusler and half-Heusler compositions that truly alloy from those that phase separate, aiding in the pursuit of reliable first-principles materials discovery.

Development of scanning probe magnetometry techniques. Over the past year, our low-temperature scanning team has achieved two primary objectives: integrating our second scanning setup into a low-temperature cryostat (LTSPM2) and improving the sensitivity of our first setup (LTSPM1) to reach previously inaccessible imaging regimes. The second scanning probe microscope, LTSPM2, is currently imaging magnetic order in an intercalated transition metal dichalcogenide ($\text{Fe}_{1/3}\text{NbS}_2$). We use this material as a testbed for magnetic imaging with LTSPM2 and explore two different strategies for imaging the antiferromagnetic order. Our first magnetic imaging strategy exploits the fact that the electrical resistance changes with the orientation of the internal magnetic domains in the material, and so we can leverage existing electrical current mapping protocols to infer the shape and size of the antiferromagnetic domains. Following the demonstration of cryo-imaging on $\text{Fe}_{1/3}\text{NbS}_2$ we will use an already integrated Razorbill strain cell to probe how strain couples to magnetic ordering in other IRG-1 materials. Our second strategy for imaging the magnetic order in this material is to look for large moments near the magnetic domain boundaries arising from uncompensated moments in a hypothetical spin-glass phase existing between antiferromagnetic boundaries. Our second objective is to improve our sensitivity from $5 \mu\text{T}/\text{Hz}^{1/2}$ to $10\text{--}50 \text{ nT}/\text{Hz}^{1/2}$ by pursuing two approaches. The first is to leverage AC magnetometry techniques such as spin-echo imaging that are substantially more sensitive than DC techniques. The second method for improving magnetic sensitivity is to utilize spin-to-charge conversion (SCC) protocols whereby the spin degree of freedom is converted to a charge degree of freedom. Finally, SCC protocols have significant improvements in sensitivity but require additional lasers of differing wavelengths. We have integrated these additional lasers and observed SCC readout.

IRG-2: Polymeric Ionic Liquids

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Overview: IRG-2 (Polymeric Ionic Liquids) seeks to advance the fundamental understanding of self-assembly, mechanics, and ion motion in polymeric materials containing ionic-liquid inspired functionalities and to impart polymer materials with triggerable properties such as photochromatism, multivalent ion conductivity, redox activity, and magnetism. These goals are addressed through advanced synthetic efforts, characterization tools, and field-theoretic simulations. The long-term outcome of this research will include fundamental insights into the structure and self-assembly of Polymeric Ionic Liquids (PILs), design rules for charge-conducting materials, and synthetic methods to create materials with exciting new properties. The following report is separated into three sections: (1) *structural studies and phase behavior of PILs*, (2) *structured PILs with high ion-conductivity*, and (3) *high-performance PILs with novel chemistries*.

Research Progress:***Structural studies and phase behavior of PILs***

Chain conformation of PIL melts. Although the conformation of a polymer is critical to nearly all its properties, the role of charged sidechains in the chain structure of PILs is unknown. IRG-2 researchers generated deuterated polymeric ionic liquids to enable small and ultra-small angle neutron scattering experiments to uncover the chain conformation of these polymers. These experiments examined the PIL in the bulk state as well as in the presence of an ionic liquid that is an analog of the PIL monomer. Although it was anticipated that the PIL would adopt an ideal (theta) conformation in the bulk state, it was instead found that the counterions are highly attracted to the backbone and swell the polymer coil. This observation has restructured the thinking about the assembly of PILs, which adopt more expanded conformations than conventional polymer science knowledge would predict.

The conformation of the PIL was also studied under solvated conditions where the PIL is blended with an IL (Fig. 5). The experimental trends show that the solvated polymers display tighter conformations at higher polymer concentrations, consistent with typical trends of the excluded volume. In aggregate, these results suggest that PILs have similar conformations to conventional polymers in semidilute conditions, but analogies to conventional polymer melts break down at high concentrations [1].

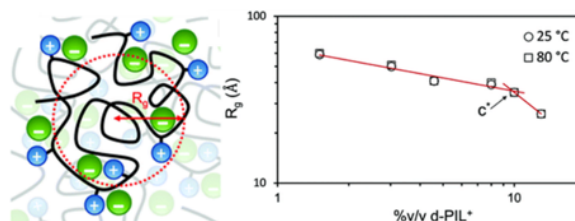


Fig. 5. For polycation PILs, R_g is determined from neutron scattering experiments in the bulk state as well as when swollen by additional IL. The R_g tends to decrease as the polymer concentration increases, suggesting that excluded volume plays a role in determining the size of these polymer chains.

Ionic compatibilization and microphase stabilization in polymeric ionic liquid blends. Electrostatic attractions can be leveraged to compatibilize blends of oppositely charged, but otherwise immiscible, polymers, resulting in a system that is either macroscopically disordered or possessing an ordered microstructure without the need for block architectures. Such electrostatically-stabilized microphase separation has been predicted theoretically but has yet to see an experimental realization. PILs are an ideal platform to design novel solid-state materials based on this principle, since their bulky pendant charges do not need to be solvated in order to render the material tractable. Using equilibrium self-consistent field theory, IRG-2 researchers explored the phase behavior of a model immiscible charged polymer blend, revealing how the phase behavior in this system can be manipulated by tuning electrostatic parameters such as charge density, salt or counterion concentration, and dielectric constant. Our theoretical model predicts that the conventional block copolymer phases can be recovered in such electrostatically-compatibilized blends, in addition to various exotic low-symmetry phases (Fig. 6). Currently, IRG-2 researchers are investigating how the structural properties of PIL blends compare with the theoretical predictions, and what the implications are for the design of materials based on electrostatic compatibilization of otherwise immiscible backbone chemistries [2].

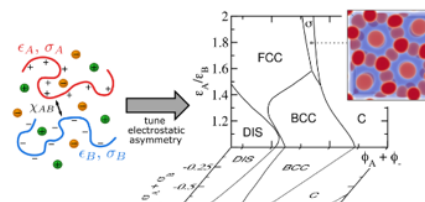


Fig. 6. SCFT phase diagram of binary blends of charged polymers, as a function of dielectric contrast ϵ_A/ϵ_B , for the charge-symmetric case. Multiple microphases are stabilized by ionic interaction.

Besides the above original research, the IRG-2 team has prepared a review article discussing state-of-the-art polysiloxane compatibilization strategies for silicone-organic polymer blends through block copolymer additives, reactive blending techniques, interpenetrating polymer networks, and polymer end-group interactions. Emphasis is placed on chemical innovation in the design of compatibilization agents that may expedite the commercialization of new silicone-organic materials. We anticipate that hybrid silicone blends will continue to play an important role in fundamental and applied materials science across industry and academia [3].

Structured PILs with high ion-conductivity

Polymeric zwitterionic solid electrolytes with superionic lithium transport. Semicrystalline zwitterionic (ZI) solid polymer electrolytes (SPEs) are a new class of materials that can mitigate many of the conventional issues associated with solid-state electrolytes. The superionically conductive crystalline domains of these materials provide a conduction mechanism similar to superionic ceramics, bypassing the conventionally limiting aspects of polymeric electrolytes (conductivity coupled to segmental relaxation, slow dynamics). IRG-2 researchers showed that facile transport is enabled by bulky cationic and anionic groups tethered to the backbone and arises from the weak interactions between lithium and framework ions. We further hypothesized that the disparity in size between lithium and constituent ions of the polymeric zwitterionic liquid (PZIL) creates sufficient free volume for the superionic transport of Li^+ . The electrochemically determined ionic conductivity of this polymer electrolyte is competitive with that of state-of-the-art polymeric ion conductors ($\sigma \approx 1.6 \text{ mS/cm}$), despite its modest T_g value ($T_g \approx 270\text{--}300 \text{ K}$). Significantly, ^7Li solid-state nuclear magnetic resonance (NMR) measurements indicate the presence of multiple lithium environments associated with different mobilities, suggesting an accelerated conductivity mode through crystalline domains. From the ^7Li and ^{19}F NMR self-diffusion coefficients obtained via pulsed field gradient NMR (PFG NMR), we calculated a lithium transport number of 0.67, which is markedly larger than the corresponding value for PEO ($t_+ \approx 0.2$). These results clearly illustrate the potential of PZILs as new design platforms for solid polymer electrolytes with superionic conduction (Fig. 7) [4].

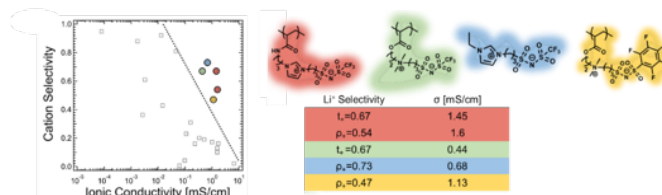


Fig. 7. When compared against data from the literature (black squares) the zwitterionic designs show marked improvements in terms of their conductivity and selectivity, beating the empirical 'upper-bound' indicated by the dotted line.

Confinement promotes proton hopping in ion-conducting block copolymer PILs. The structure of PILs is also important in proton conduction. Proton-conducting polymer membranes frequently contain nanoscale structural and ion-conducting phases. In addition to enhancing the mechanical properties, the nanoscale structure often leads to a significant increase in ion dynamics; however, the molecular underpinnings behind this phenomenon are not well understood. IRG-2 researchers synthesized a model proton-conducting PIL block copolymer, polystyrene-*block*-poly(5-aminoethylimidazolium acrylamide) TFSI (PS-*b*-PIL), which formed a lamella bulk morphology, increasing the proton conductivity up to an order of magnitude higher than an analogous homopolymer (Fig. 8). Variable temperature ^1H solid-state magic angle spinning (MAS) NMR spectroscopy also revealed that confinement in the block copolymer PIL decreases the segmental motion of the PIL and increases the structural rigidity of the ionic functional groups. This increased structural rigidity is found to dramatically increase the connectivity of the hydrogen bonding network in the block copolymer PIL according to double quantum–single quantum ^1H MAS NMR. This nanoscale restructuring leads to a significant increase in Grotthuss proton hopping dynamics in the block copolymer PIL compared to the homopolymer. As the demand for anhydrous proton conducting materials increases, these results elucidate new design rules for the use of nanostructuring to simultaneously enhance both mechanical properties and proton conductivity [5].

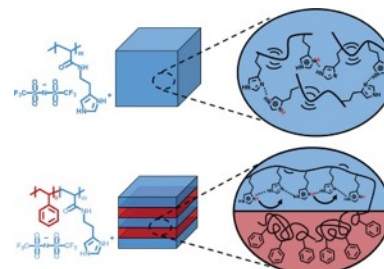


Fig. 8. Confinement in block copolymer PIL increases the structural rigidity while also increases the hydrogen bonding network, promoting proton hopping dynamics.

The IRG-2 team also prepared a review article discussing electronic, ionic, and mixed conduction in polymeric systems. To explore whether ion conductivity comes at the cost of electronic conductivity, we reviewed the fundamental mechanisms related to electronic and ionic conduction and ways by which they are coupled in polymeric mixed conductors (Fig. 9). By identifying constraints on the design of mixed conductors and unique behaviors arising from electron and ion-coupling in polymers, we highlighted next steps toward developing design rules unique to polymeric mixed conductors [6].

High-performance PILs with novel chemistries

Electron-deficient imidazoles in solid-state polymer electrolytes. Solid-state polymer electrolytes offer a safer alternative to traditional lithium-ion batteries based on organic electrolytes. IRG-2 researchers systematically investigated poly(methylsiloxane) polymers functionalized with a series of halogen-substituted imidazoles (Fig. 10) and showed that Li^+ ion transport numbers can be tuned by an electron-deficient heterocycle ligand as measured by pulsed-field-gradient nuclear magnetic resonance (PFG NMR) and NMR relaxometry. In addition to the electronic properties, the steric properties of imidazole ligands were shown to affect the Li^+ ion transport and the total ionic conductivity. Although beneficial for Li^+ transport, electron-deficient Im ligands result in clustering, as indicated by wide-angle X-ray scattering, and poor salt dissolution, which in turn impedes the overall ionic transport. This work highlighted the importance of synthetic design and the necessity for high salt solvation and weak cation-polymer binding to obtain high Li^+ transport numbers [7].

Optimum in ligand density for conductivity in polymer electrolytes. Ligand density is also of importance in controlling the ionic conductivity. In a family of imidazole side chain grafted siloxane polymer electrolytes containing LiTFSI, we concluded that while the presence of imidazole solvation sites promotes solubilization of Li^+ containing salts, it is not necessary to substitute every monomer in the polymer design. Rather, optimization of Li^+ conductivity relies on a balance between imidazole presence and the ability of the chains to rearrange locally to facilitate transport. Lowering the imidazole content in the ethane-imidazole series leads to a 10-fold increase in conductivity, while conductivity decreases for the phenyl-imidazole series due to differences in steric bulk (Fig. 11). These results emphasize the importance of local re-arrangements in facilitating ion transport at low solvation site density, confirming the role of dynamic percolation, and suggest that an optimum ligand density exists for improved charge transport [8].

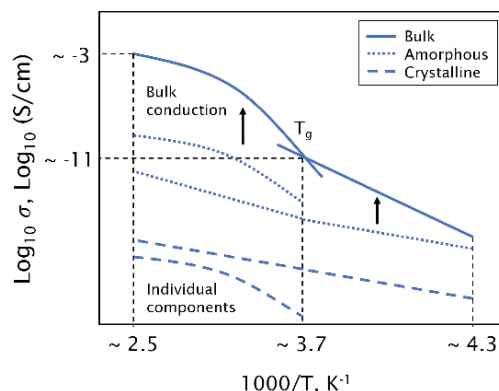


Fig. 9. Semicrystalline mixed conductors exhibit ionic conduction across both their crystalline and amorphous domains. We highlight that this leads to transport in both domains, with segmental motion-mediated ion transport and Arrhenius-type ion hopping contributing in each to the experimentally measured bulk ionic conductivity.

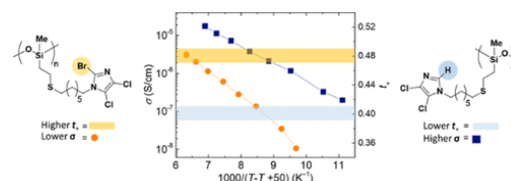


Fig. 10. Electron-deficient ligands benefit Li^+ transport while suffer from low ionic conductivity due to insufficient salt dissolution.

Database creation, visualization, and statistical learning for polymer Li⁺-electrolyte design. IRG-2 researchers described the curation and analysis of a database of polymer Li⁺-electrolyte conductivity performance, manually extracted from the published literature. We focused on solid, dry polymer electrolytes without additives. Data were extracted from 65 publications, resulting in 655 unique polymer-anion-salt concentration entries and 5225 individual conductivity data points to create an interactive database: PEDatamine.org. Visualization of the collective data set suggested that individual features, other than the activation energy, are poor predictors of conductivity performance across the wide range of polymer chemistries, Li salts, and salt concentrations examined. Such open-access web-based visualization will enable additional trends to be explored by other researchers in the field, further expanding the utility of the curated experimental database [9].

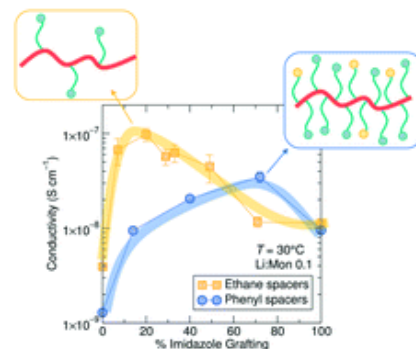


Fig. 11. Different optimal ligand densities for two functional imidazole series indicate a large design space to maximize ionic conductivity of PILs.

Multiwavelength photodetectors based on an azobenzene PIL.

Organic photodetectors (OPDs) are a promising class of light-detecting devices that can be created with simple fabrication techniques from a large variety of chemical building blocks. Here, we report the development and characterization of a bilayer azobenzene polymeric ionic liquid-based photodetector with multiwavelength sensing capabilities. The photoresponsive azobenzene PIL (Azo-PIL) was designed such that it would have opposite solubility to the semiconducting polymer, PhF-2,3, which facilitates device fabrication by spin-coating. Once incorporated into the photodetector, both ultraviolet (UV) and visible light induce a 10^2 – 10^3 increase in current at a constant voltage within 10 s, which decays immediately when the light is turned off (Fig. 12). This light-mediated performance is fatigue-resistant across multiple ON/OFF cycles and can be modulated with wavelengths far into the visible region (660 and 700 nm). Frontier energy level calculations of the light-induced charge carrier density indicate that this light-responsive increase in current is due to photoexcitation and a subsequent charge-transfer process between the azobenzene polymeric ionic liquid and the semiconducting polymer [10].

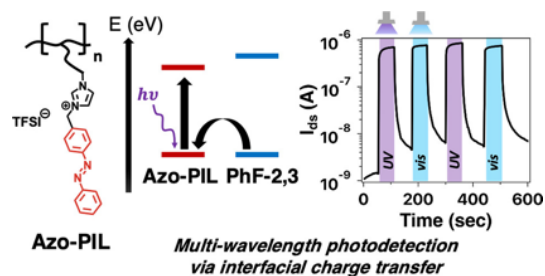


Fig. 12. The device based on bilayers of azobenzene PIL exhibits sensing capabilities for multiple wavelengths of light corresponding with the azobenzene absorption profile.

Future Plans:

We will continue to probe the structure–property relationships that underpin Zwitterions with (super)ionic conductivity in novel polymer electrolytes. Efforts in the next year will connect the chemistry of Zwitterions and charge density along a polymer backbone with crystallite structure, size, and shape. These insights will help unravel the fundamental contributions to (super)ionic conductivity and limits of performance that are expected to be crucial in the design of advanced materials. The IRG-2 team will continue to study the fundamental chemistry and physics of ion-containing polymers. One important direction that warrants further research is the ability of ions to compatibilize polymer blends which otherwise phase separate. We will investigate the impact of charge density and placement in the compatibilization of polymer blends using model systems to control charge chemistry, placement, and density. These efforts will lay the groundwork necessary to investigate compatibilization effects in commercially relevant materials, for example, polyolefins and semiconducting polymers.

IRG-3: Resilient Multiphase Soft Materials

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Overview: The materials challenge addressed in IRG3 is to understand and develop new syntheses, processing schemes, and structure-property relationships for resilient, multi-phase soft materials. We seek to characterize how nature uses non-equilibrium assembly and phase transformation to create multi-phase materials with carefully controlled morphologies, interphases and interfaces across a hierarchy of length scales, understand how such structuring achieves superior mechanical performance, and translate these aspects to new synthetic materials and processing methods. IRG3 Research in the current reporting period falls along three themes: *(i)* bioinspired chemistries for functional materials, *(ii)* understanding and controlling non-equilibrium processing, and *(iii)* mechanics of natural and bio-inspired materials.

Research Progress:

Innovations in bioinspired chemistries for functional materials. IRG members continue to advance numerous synthetic approaches for the development of resilient multiphase soft materials, including a variety of click chemistry strategies [1], and photoactive chemistries [2]. These advances in turn enable the design of novel materials, including switchable coatings and materials for actuation. In one recent study, the solution thermodynamics and play important roles in the modification of a wide variety of consumer products, where viscosity rheology of topology-

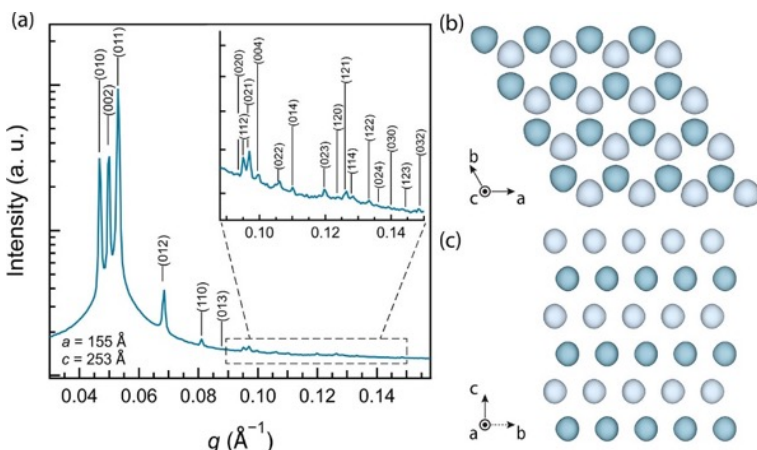


Fig. 13. (a) Representative SAXS data for a F4DF triblock copolymer containing poly(2,2,2-trifluoroethyl acrylate)-*block*-poly(4-dodecyl acrylate)-*block*-poly(2,2,2-trifluoroethyl acrylate). This material forms a pure HCP sphere phase after thermal annealing at 120 °C for 14 h. (b,c) Unit cell electron density reconstruction along two axes [4].

for the degree of coil expansion and viscosity modification, it was found that increased branching significantly enhances polymer-polymer interactions even under dilute conditions, providing potential guidelines for how chain topology can be used to tune solution phase behavior in more concentrated systems. Building on their expertise in the design of block copolymer synthesis and control of molar mass dispersity, IRG members also reported the discovery of a stable and pure hexagonally close-packed (HCP) phase in linear block copolymer melts formed without the use of blending or other complex processing techniques (**Fig. 13**) [4]. Finally, IRG members interrogated the role of molecular context of Dopa in peptide adsorption and adhesive performance [5]. Using both experiment and replica-exchange and umbrella-sampling molecular dynamics simulations, they demonstrated the importance of chemical character of the target surface and proximity of cationic and hydrophobic residues to 3,4-dihydroxyphenylalanine (Dopa), a post-translationally modified variant of tyrosine. These results will guide the development of peptide-based underwater adhesives.

Innovations in understanding and controlling non-equilibrium processing. IRG-3 research continues to advance fundamental understanding as well as engineering, simulation and analysis tools for processing bioinspired multi-phase soft materials. For example, a recent review highlighted the multi-scale simulation tools developed within the IRG for understanding the structure, interactions and assembly of intrinsically disordered proteins and other macromolecules [6]. These tools were recently applied to understand coacervate-driven liquid-liquid phase separation (LLPS) of tau protein and its modification through interactions with RNA and polyethylene glycol (PEG) additives [7]. By combining fully atomistic simulations to resolve molecular conformations with field theoretic simulations to realize sufficiently large systems to observe the formation of coacervate droplets, IRG researchers were able to identify how specific tau-RNA interactions and macromolecular crowding drive a competition between single-component coacervation of tau and complex coacervation of tau-RNA complexes to produce immiscible coacervates with divergent properties (**Fig. 14**). The simulations were in qualitative agreement with experiments, which found that the coexistence of the separate coacervate phases is stabilized by large rheological contrast between the simple and complex coacervate droplets. These results provide new understanding for the development of internally structured coacervates in biomolecular condensates, and guidelines for how these designs could be translated to synthetic materials.

defined poly(meth)acrylate-based polymers were investigated [3]. Such polymers control must be balanced with mechanical stability. Using temperature-dependent viscosity measurements, dynamic light scattering (DLS), and small-angle neutron scattering (SANS), IRG members studied the influence of topology on the temperature-induced swelling and viscosity modification of industrially relevant poly(stearyl methacrylate-*co*-methyl methacrylate) [p(SMA-*co*-MMA)] polymers with various architectures including linear, randomly branched, and star-shaped topologies. In addition to expected trends

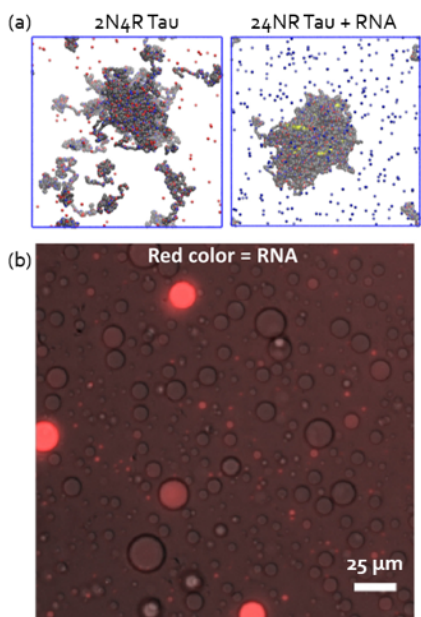


Fig. 14. (a) Atomistic simulations of Tau cocervates formed with (left) and without (right) RNA (yellow) indicating significant differences in conformation upon complex cocervation. (b) Fluorescence micrograph indicating coexistence of immiscible cocervate droplets of simple Tau cocervate (low fluorescence) and complex Tau-RNA cocervate (high fluorescence). Adapted from [7].

Along these lines, IRG researchers have merged their understanding for the role of internally structured coacervate chemistries in marine adhesive materials with synthetic schemes for polymeric ionic liquids (PILs) developed in IRG-2 to design self-coacervating peptide-mimetic PILs containing moieties that encode cation- π interactions. Structural and mechanical characterization revealed that the specific incorporation of cation- π interactions simultaneously imbues coacervates with internal structure and instantly-forming adhesive properties, not unlike those found in mussel foot adhesive proteins [8]. Researchers leveraged these remarkable properties to demonstrate the use of cation- π functionalized PILs as versatile, rapidly setting, highly tough adhesives for application to substrates across a range of surface chemistries. This study emphasizes the significant advances in material design and performance that can be achieved by learning the motifs of chemistry and processing utilized in resilient natural materials, and applying them for the design of exceptionally-performing engineered synthetic materials. Inspired by these developments, IRG researchers have also designed microfluidic devices to control the mixing, processing and dispensing of bio-inspired coacervate materials. Specifically, researchers have developed novel 3D printing schemes and workflows for the rapid prototyping of microfluidic chips, and have used them fabricate microfluidic herringbone devices to achieve rapid yet controlled laminar mixing of polyelectrolyte streams [9].

Innovations in the mechanics of natural and bioinspired materials. IRG researchers continue to develop new insights into the stiffness, strength, and failure of multiphase materials through experiment, theory and computation. In studies focused on natural materials, researchers examined the advantages of the cure-in-place manufacturing capabilities of marine mussels to adhere to roughened and curved surfaces, as well as the role of suction in strengthening the adhesive joint [10-11]. In studies of swell shark egg cases, one of the toughest membranes known, IRG researchers established the importance of a nanolattice architecture that provides mechanical toughness and reinforcement, while enabling permeability [12]. These discoveries provide fundamental insights for the improvement of multifunctional, fiber-reinforced soft composites, and mechanical metamaterials.

IRG researchers also examined the influence of viscoelasticity on crack propagation in a soft material to settle a longstanding controversy between two competing models by Knauss-Schapery and deGennes respectively that describe nonlinear dependence of the speed of crack extension on applied load. IRG researchers showed that the two models are essentially equivalent for viscoelastic crack propagation and the standard description that the toughness of the material is essentially rate independent, and the rate dependence of the fracture process arises from viscoelastic interactions of the viscoelastic body and the process zone holds [13]. Researchers also analyzed crack propagation at the interface between a viscoelastic material and a linear elastic material, with direct relevance to infiltrated or filled polymer composites [14]. Experimental studies of interfacial mechanics included investigations of the roles of geometry and surface chemistries on the mechanics of hydrogel interfaces, including the solvophilic transition in amphiphilic hydrogels in mechanical and adhesive performance [15-17].

In one particularly exciting example, the abilities of IRG members to combine synergistic advances in synthesis, processing, and mechanics has enabled the development of tough 3D printed polymer composites. Through use of wavelength-selective curing of custom resins, IRG members produced multimaterial objects formed from two interpenetrated polymer networks with tough, well-defined interfaces between chemically distinct domains (Fig. 15) [18]. Using printed test structures, interfaces were characterized through spatial resolution of their chemical composition, localized mechanical properties, and bulk fracture strength and were shown to outperform those produced by traditional printing methods. Researchers also demonstrated the facile, on-demand manufacturing of thermally activated polymer foams with desirable properties such as mechanical strength, controlled porosity, and varied composition [19]. Key to the success of this process is the incorporation of photopolymerizable monomers (matrix) and thermally expandable microspheres (foaming agent) use of two-step curing with 3D photopolymerization and subsequent thermal processing, to produce microporosity throughout the resulting polymer network. Low-density foams with a porosity up to 85% increased specific modulus and energy dissipation when compared to the bulk matrix were demonstrated. These new approaches to the additive manufacturing of graded and multimaterial polymer composites opens exciting new opportunities to create geometrically and chemical complex materials to enhance mechanical performance.

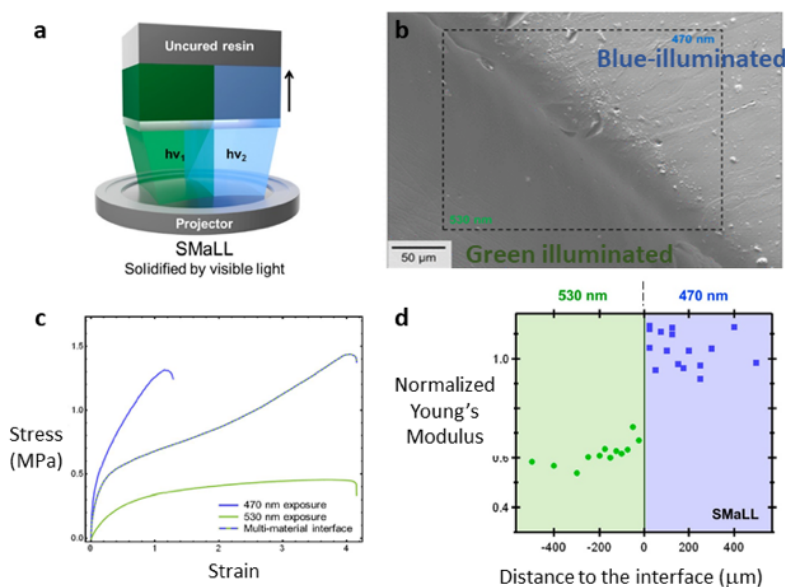


Fig. 15. (a) Schematic showing the wavelength-specific multimaterial printing. (b) SEM micrograph showing interface between green and blue-illuminated regions, with differing surface roughness and clean boundary. (c) Stress-strain data for the single phase and multiphase materials showing that the composite material retains both the enhanced stiffness and enhanced strain at failure observed in the individual phases. (d) Young's modulus as a function of distance to the interface shows the distinct mechanical phases and sharp nature of the interface. Adapted from [18].

Future Plans:

Synthesis of covalent adaptable networks (CANs) as a sustainable alternative to thermosets. CANs hold promise as a (re)processable and chemically recyclable alternative to traditional thermosets due to their stimuli-responsive and reversible crosslinks. In detail, synthetically accessible bicyclo[3.3.1]nonane (BCN) bis-alkyl halide monomer units containing a sulfur internal nucleophile are used to crosslink pyridine-functionalized linear polymers. The specific incorporation of a sulfur at the bridgehead positions, allows neighboring group participation (NGP) to be exploited in lieu of catalysts to dramatically increase the rate of crosslinker bond exchange (Fig. 16). As a result, dynamic exchange leads to an Arrhenius-dependence on viscous flow at elevated temperatures (130–170 °C). This thermally mediated bond exchange and flow behavior can be harnessed to regenerate percolating ionic networks over multiple (re)processing cycles, addressing key criteria for the ultimate goal of developing thermosets with extended lifecycles.

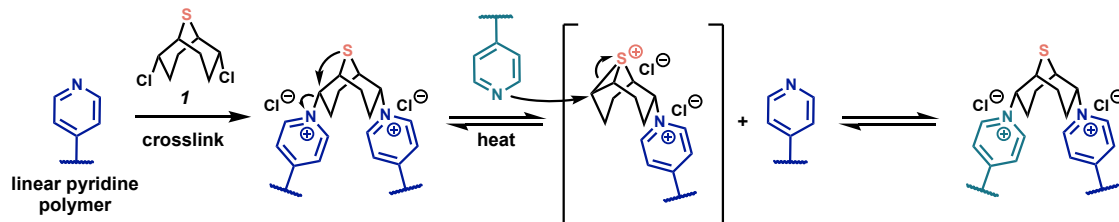


Fig. 16. Schematic of CAN synthetic strategy.

Non-equilibrium processing of multi-phase coacervate materials from sequence-defined chemistries.

We plan to integrate separate past successes in developing synthetic chemistries for sequence-defined polymers, measurement and modeling tools to understand coacervation and LLPS in bio/macromolecular materials, and new fluidic and printing devices for complex structured materials to demonstrate how understanding and abilities across these efforts can be combined to create materials with novel architecture. In particular, we hope to investigate how combinations of *in situ* bioinspired reactive chemistries (e.g. metal-ligand coordination complexation) and/or competing intermolecular interactions (e.g. folded secondary structure and mesoscale assembly) encoded by chemical sequence can be used to produce coacervating materials with potentially novel properties due to arrested non-equilibrium, multi-phase structures. In particular, we will utilize recently developed microfluidic fabrication tools [9] and microrheology characterization tools [20] to study the how flow and mass transport phenomena can be used to control whether, where and how arrest occurs within a developing coacervate material to achieve potentially novel morphologies and architectures. We will also use these capabilities to devise schemes whereby native protein coacervation and crosslinking (such as those found in processing of the *Glycera* jaw) can be integrated with familiar processes for the production of polymeric materials (e.g. interfacial polymerization) to develop new routes to protein-based materials as potential alternatives to synthetic analogues with competitive or superior mechanical properties.

Mechanics of hierarchically porous and composite soft materials. IRG members continue to advance the integration of micro-scale structuring approaches and additive manufacturing to create hierarchical multi-phase soft materials, including heterogeneous and dynamically bonded hydrogels. Our ability to print porous polymer composites using thermally-expandable microspheres to printing resins will be extended to create gradient structures and complex geometries to understand how mechanical resilience can be improved as compared to traditional foaming techniques. Additionally, we are exploring the use of colloidal templating to create liquid-filled elastomeric materials both for foundational studies of material mechanics, and to provide an alternate path to porous foam manufacturing.

iSuperSeed2: Shape from Activity-Driven Folding: A Path to Materials Morphogenesis

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 Zvonimir Dogic Physics
 Mark Bowick KITP
 Sebastian Streichan Physics

iSuperSeed Postdocs: Itamar Kolvin, Zhihong You

Overview: iSuperSeed is focused on understanding how *active* processes at the molecular scale control the organization of living and bioinspired matter, and applying this understanding to the design of self-shaping materials. Significant accomplishments have been made in three complementary directions: (i) the understanding of how active stresses reconfigure soft deformable interfaces in phase separating polymer mixtures; (ii) correlating cellular structure to limb morphogenesis using in *in vivo* developing embryos; (iii) controlling the folding of stem cell sheets into 3D organoids of specific target shape.

Research Progress:

Active liquid-liquid phase separation (LLPS). Binary liquids ubiquitously exhibit LLPS. Controlling LLPS and the associated soft interfaces has numerous applications throughout materials science and engineering, such as the formation of emulsions and microphase separated lamellar phases. LLPS has also been recognized as a fundamental organizing principle in cell biology. Dogic and Kolvin developed a model experimental system for controlled studies of how active processes affect LLPS. They combined a microtubule (MT)-based active fluid with an immiscible binary polymer mixture of poly(ethylene glycol) (PEG) and Dextran. All the protein components of the MT-based active fluid partition into the Dextran phase, where they exhibit autonomous flows similar to those previously studied in the Dogic lab. PEG/Dextran interfaces have ultra-low interfacial tension, which allows for the coupling of the MT-generated active stresses to the interfacial deformations. Using a variety of imaging tools, they demonstrated that this system exhibits diverse phenomena including (1) giant interfacial fluctuations visible by the naked eye, (2) propagating waves in a non-inertial regime (**Fig. 17**), (3) active wetting transitions in which the active fluid works against gravity and climbs the chamber walls, (4) and activity-arrested phase separation, wherein the internally generate flows suppress the droplet coarsening yielding a unique non-equilibrium steady-state consisting of finite-sized reconfigurable droplets that continuously merge and break apart. To gain quantitative insight, Marchetti and You developed a versatile theoretical model of active-LLPS. The starting point is a widely-used continuum model of active liquid crystals, which describes MT-based active fluids in terms of flow velocity and nematic order parameter. To capture the interfacial dynamics, they employed a Volume-of-Fluid (VOF) approach that couples the hydrodynamics of the active fluid to that of a coexisting passive fluid through a scalar field defined to be 1 in the active phase and 0 in the passive one. The scalar field is advected by flow and keeps track of the interface dynamics. The computational model explains all of the experimentally observed features suggesting the universal nature of the observed phenomena. This combined experimental and theoretical work has been submitted for publication and is currently under review.

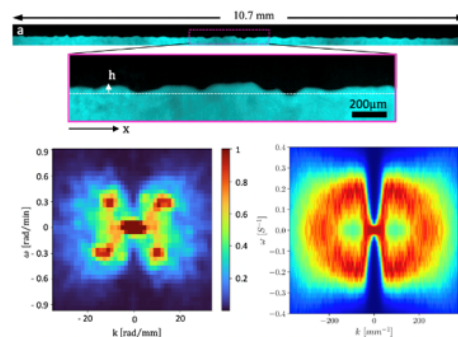


Fig. 17. Active interfaces support traveling waves, as evident from the dynamic structure factor from experiments (left) and theory (right) in the bottom row.

Connecting tissue structure to morphogenetic events in developing embryos. A central challenge of morphogenesis, the process by which tissues get in shape, is to establish the body plan of animals that determines the location of limbs and organs as the embryo grows. This problem received a great deal of attention in advanced genetic model organisms such as the fruit fly *D. Melanogaster*, uncovering insights of

how biochemical gradients establish patterning cascades that determine cell fates. *Drosophila* is an *indirect* developer, and limbs develop within the pupa at a completely different stage of development than when the fate patterns are laid down. *Direct* developers face an added challenge as they need to determine fates and develop the proper shape at the same time. As the embryo develops, direct developers typically assemble limbs in a sequential

fashion, which requires coordination across the limbs. Bowick and Streichan investigated direct limb morphogenesis in the crustacean model organism *P. Hawaiiensis*. Combining light sheet microscopy with computational analysis and physical modeling they showed that cell divisions are the main drivers of tissue flow leading to a fourfold orientationally ordered phase. Waves of anisotropic cell proliferation propagate across the embryo with precise choreography, such that defects introduced into the nascent lattice by cell divisions are healed by subsequent divisions through active defect climb (Fig. 18). Orchestrating cell proliferation rates and orientations enables cell divisions to organize, rather than fluidize, the tissue. The result is a robust, active mechanism for generating global orientational order in a non-equilibrium system that sets the stage for the subsequent limb development of shape and form. While well-known in the condensed matter community orientationally-ordered phases are less explored in biological systems [1].

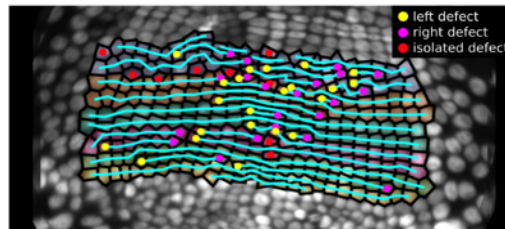


Fig. 18. Defects introduced in rows of cells by division.

Towards targeted stem cell colony folding in 3D. Stem cells are an exciting material to study both the differentiation of cells, as well as fundamental aspects of morphogenesis. Streichan and Karzbrun addressed the problem of culturing in 3D stem cells environment to establish organoids of well-defined shape, volume, and cell density. We refer to these organoids as clean slate, as these cells remain stem cells, and should be able to differentiate according to biochemical signals. Our first approach consisted of seeding planar stem cell culture on a dish with triangle, square, rectangle, and circle 2D shapes coated with extracellular matrix proteins, such as Laminin, that promote stem cell culture adhesion. This generated 2D cell sheets of defined shape. The next step consists of doping media with a low concentration of matrigel, a commercially available collagen rich gel. Seven hours after matrigel supply, we note the stem cell colony undergoes a folding transition. The tissue initiates folding from the boundary, such that the boundary continues shrinking, akin to a purse string. Eventually, the stem cell tissue will be completely closed around a single lumen, which then inflates into a curved sheet surrounding a single lumen (Fig. 19). The 2D pattern sets the final shape of the curved tissue: A triangle becomes a pyramid, while a rectangle turns into a cylinder. The micropatterning technique scales well, allowing for the establishment of hundreds such stem cell cultures within the same petridish. Segmentation shows that we have succeeded with setting stem cell density independent of the initial pattern shape or area. This work is nearing completion and will soon be submitted.

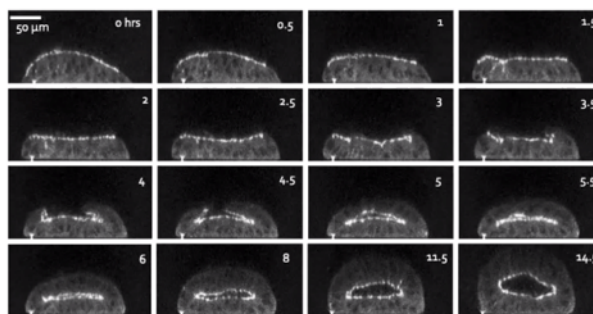


Fig. 19. Sequential formation of a 3D stem cell lumenoid from an initial patterned 2D cell sheet.

iSuperseed: Pathways to the Workforce 2021: A Workshop in Leadership, Communication, and Professional Competencies

Dorothy Pak UC Santa Barbara
Christine Morrow University of Colorado Boulder

Overview: This workshop addresses the NSF INCLUDES Big Idea around developing STEM talent from all sectors of society. The Pathways workshop's goals were to bring together a diverse group of students and post-docs in order to address building their professional networks, sharpening their oral and written communication skills, and integrating entrepreneurship with their technical knowledge. The workshop was organized and implemented through the efforts of MRSEC Education Directors Christine Morrow (CU Boulder) and Dotti Pak (UCSB) and ran remotely from August 8–10, 2021.

Participant Information: Workshop participants were recruited from MRSECs and PREMs and students who participated in recent years as REUs at a MRSEC or PREM. Participants were selected based on their interest in Materials Science, their leadership qualities, and a demonstrated interest in developing communication and entrepreneurial skills. The workshop was offered at no cost to the participants. There were 33 participants from 19 different home institutions across the contiguous United States and Puerto Rico, including 13 undergraduates, 18 graduate students and 2 postdocs. Demographics included 42% female and 42% URM participants.

Workshop Program: Morrow and Pak researched, planned and organized the program paying careful attention to recruiting and retaining a diverse group of expert speakers with talks and activities that aligned with the workshop's goals. We assembled a student advisory board from 2019 Pathways participants, who advised us on scheduling, speakers, and the logistics of remote presentation. Two of the 2019 presenters (Kayla Nguyen, U Illinois and Gary Beall, Texas State) agreed to repeat, along with Asmeret Berhe (UC Merced), Allison Mattheis (Cal State LA), Patricia Rankin (CU Boulder), Sarabeth Berk (Morethanmytitle.com), Allison Hatt (PNNL) and a career panel of graduate students and recent graduate students.

Evaluative Feedback: At the end of each day, participants offered anonymous feedback in real time using the Poll Everywhere smartphone app or a web browser. Morrow and Pak developed the survey questions drawing from their experience with a variety of workshops they have conducted during their tenure as MRSEC Education Directors. The participants' responses and comments were used to assess the workshop's effectiveness and to identify areas of improvement. Overall, participants responded very favorably to the workshop.

Future Plans: In response to participant feedback, the third and final Pathways to the Workforce workshop will be a student-run inter MRSEC and PREM conference for graduate students to be held at Ohio State on October 12–14, 2022.

Seed: Selecting for Phase-Separating Nucleic Acid Coacervates

Omar Saleh

Materials and Biomolecular Science and Engineering

Seed Affiliates: Irene Chen (UC Los Angeles)**Seed Graduate Students:** Anna Nguyen (BMSE), Nate Conrad (Physics)

Overview: We are leveraging tools of sequence-specific DNA assembly and DNA biochemistry to discover rules for the formation of complex coacervates. Complex coacervation involves the condensation of a dense liquid phase from a macromolecular solution, typically driven by counterion release upon binding of oppositely-charged macromolecules, though in DNA systems, base-pairing can also play a role (as shown in our prior work [1]). Given their negative charge, nucleic acids are optimal constituents of such processes. Factors other than net charge are important for coacervation; using DNA, we can easily explore parameters such as macromolecular rigidity, shape, and charge density.

Research Progress: We have studied the phase separation tendency of DNA molecules of various structures when complexed with a 40-unit polylysine. We have designed a set of 7 basic DNA structures, all with the same charge, but with very different shapes and flexibilities. Phase separation is judged by turbidity and microscopy (**Fig. 20A**). We have found an unexpected non-monotonic behavior in which increasing the DNA rigidity first decreases, then increases, the tendency to phase separate. This is likely due to competition between charge density (which favors phase separation) and rigidity (which disfavors it). Confirmation of this unexpected phase behavior can be found by visualizing multi-phase droplets (**Fig. 20A**), which indeed show separation (immiscibility) of distinct phases that differ in the rigidity of the constituent DNA. In a methods-development effort, we have invented a way to more rapidly measure phase behavior by encapsulating coacervate droplets within water-in-oil emulsions (**Fig. 20B**), where precision image-based measurement of relative volumes quickly elucidates the phase diagram through application of the lever rule (**Fig. 20C**).

Other outcomes: Materials substrates developed here are impacting the Saleh lab's Keck- and NSF-funded project on DNA based coacervates, as well as providing data to support ongoing grant applications. Saleh's work on this system has led him to recently become formally affiliated with the BioPACIFIC MIP.

Future Plans: As this seed grant winds down, our major goal is to finalize and publish the two experiments discussed above.

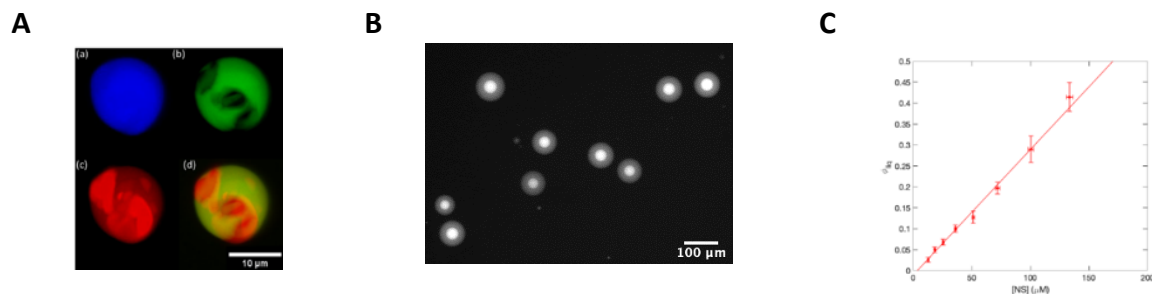


Fig. 20. (A) Multi-color fluorescent images of multiphase electrostatic coacervate formed by mixing polylysine (a; blue), flexible single-stranded DNA (b; green), and rigid double-stranded DNA (c; red). The composite image (d) shows the mutual immiscibility of the two types of DNA. (B) Image of liquid droplets of DNA within water-in-oil emulsion droplets. (C) Analysis of images, such as in (B), demonstrate applicability of the lever rule to this phase behavior, thus permitting direct estimate of binodal phase boundaries from the slope and x intercept of the plotted volume fraction, ϕ , vs. concentration curve.

Seed: Electronic Structure and Scattering Mechanisms in Twisted Bilayer Graphene

Vojtech Vlcek

Chem. & Biochem.

Andrea F. Young

Physics

Seed Graduate Student: Marec Serlin Seed Postdoc: Mariya Romanova

Research Progress. In 2021, we finalized the study of the twisted bilayers of graphene under compression and published our research in *npj Computational Materials* [1]. The numerical work greatly expanded the toolkit of stochastic many-body computational methods, which enabled calculations for a giant moiré system.

In detail, we studied a lesser-explored avenue to achieve strong localization of electronic states through applying compression. Twisted bilayer graphene exhibits all hallmarks of strong electronic correlations under specific conditions governed by the mutual twist of the two (otherwise weakly correlated) monolayers of graphene. At the magic angle twist, the mutual coupling leads to the formation of flat bands which localize electrons, but, simultaneously, the weakly correlated electronic states suppress the mutual Coulombic interactions. This leads to a competition between kinetic energy and repulsive electron-electron terms. The regime is associated with the onset of interesting physical phenomena. Increased coupling of two monolayers can be controlled (besides the twist angle) by decreasing the interlayer distance. Indeed, this leads to the localization of electrons near the Fermi level. The corresponding states are confined to a narrow region near the AA stacking of the bilayer (see Fig. 21).

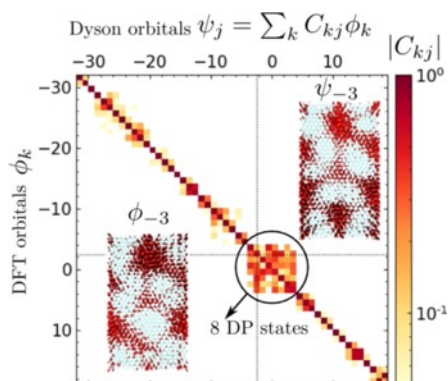


Fig. 21. Coefficient matrix obtained from the exact diagonalization of quasiparticle Hamiltonian in the subspace of states within 0.5 eV near the Fermi level (results for the pressure of 100 GPa). With a black circle, we indicate 8 Dirac point states that are quasi-degenerate in energy and that represent a correlated region. Inset: We plot a density of state 3 to compare a KS orbital to the QP orbital – both are showing strong localization in the AA stacking region of the twisted bilayer. State 3 is highlighted with a dotted line in the figure. The figure is taken from Ref [1].

We identified the subspace of correlated electrons using the self-consistent diagrammatic many-body approach by investigating the eigenstates of the quasiparticle Hamiltonian (see Figure 1). By comparing to the available experimental data, we showed that our computational techniques are truly predictive (with differences being merely 10 meV with respect to photoemission spectra). Using the dynamical Hamiltonian downfolding, we investigated the dynamical correlations due to the weakly correlated electrons, which renormalize the Coulomb interactions in the flat bands. The results demonstrate that the screening increases with electron localization under pressure, but it does not appreciably alter the mutual electron-electron interactions. As a result, we document the formation of strongly interacting states, which are likely associated with robust insulating behavior. In contrast to the twisted bilayer graphene near the magic angle conditions, the mechanism of interlayer coupling is distinct. Our study suggests that compression is a significantly different route in deterministic manipulation of quantum interactions in moiré systems.

Seed: Understanding Thermal Effects on the Microstructure of Additive-Manufactured Materials

Yangying Zhu Mechanical Engineering

Seed Affiliates: Tresa Pollock (UC Santa Barbara), Raphaële Clément (UC Santa Barbara)**Seed Graduate Students:** Olivia Wander (Materials, NSF GRFP), Vijay Kumar (Mechanical Engineering)

Overview: The main goals of this seed project are to probe and understand how localized and dynamic heating and cooling affect the microstructure of additive manufactured (AM) materials, and optimize AM processes by tuning thermal interfacial resistance. During selective laser melting (SLM), temperature gradients and rates will be probed operando using a high-speed infrared (IR) camera, while grain growth and microstructure will be characterized ex situ with electron microscopy and diffraction. Using machine learning, a correlation between the thermal and materials properties will be established, which allows us to tune AM processes by precisely controlling the temperature field.

Research Progress: We have first designed a custom argon (Ar) chamber (**Fig. 22a**) with laser access and a viewport for a high-speed IR camera (M3K, Telops). The chamber will be built and mounted to a metal SLM printer (Aconity Mini) in Tresa Pollock's lab at UCSB. The viewing angle of the IR camera and its working distance to the powder bed are optimized to achieve maximum spatial resolution (30 μm per pixel) and a reasonable field-of-view (1 mm \times 9 mm). Next, we have established a protocol to calibrate the emissivity of CoNi 131349 powders, the material to be printed, at various temperatures in an Ar environment using a precision temperature stage with an IR-transparent window. An example of CoNi powders uniformly heated to 270 $^{\circ}\text{C}$ is shown in **Fig. 22b**. The calibration step is important to ensure the accuracy of temperature measurement since IR camera only measures the thermal radiation whereas the temperature is further determined by the emissivity of the sample. The result (**Fig. 22c**) clearly illustrates temperature dependence of the emissivity of CoNi 131349 in the range of 100-400 $^{\circ}\text{C}$ in an inert environment, which necessitates further experiments to extend the calibration temperature to the melting point. Furthermore, we developed Matlab codes to automatically extract temperature gradients (dT/dx) in an arbitrary direction and transient temperature rates (dT/dt) from IR videos.

Other Outcomes: The IR imaging calibration protocol developed in this seed has led to an ONR grant to Zhu to study flow boiling in microchannels. The technique will also be leveraged in Zhu's NSF CAREER project to validate Raman thermography measurements.

Future Plans: We will finish machining the Ar chamber and perform IR measurements to generate temperature maps of the heat impacted region. We will extend emissivity calibration to the melting point of CoNi 131349 powders to obtain accurate temperature maps, and characterize the materials microstructures. We will tune laser parameters to generate wide temperature conditions and establish a correlation with the resulting materials microstructures.

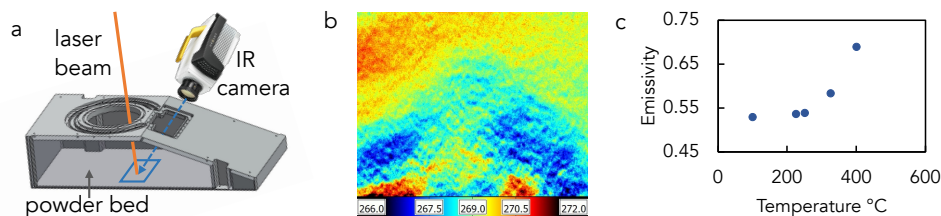


Fig. 22. (a) CAD drawing of a custom aluminum chamber interfacing a laser beam for SLM and an IR camera. (b) Temperature of CoNi 131349 powders uniformly heated to 270 $^{\circ}\text{C}$. (c) The emissivity of CoNi 131349 powders as a function of temperature.

Seed: Stereochemically Well-Defined Polymeric Materials via Biocatalytic Polymerization

Yang Yang

Chem. & Biochem.

Overview: Owing to its operational simplicity and excellent control over molecular weight and polydispersity, radical polymerization represents a powerful tool in polymer chemistry, but stereocontrol has eluded polymer chemists for decades. In transition metal-catalyzed living radical polymerization such as atom transfer radical polymerization (ATRP), the nascent radical species rapidly diffuses away from the transition-metal center, thereby precluding stereocontrol over the radical addition step. Given the importance of polymer stereochemistry in determining diverse properties, new methods for tacticity-controlled radical polymerization will achieve novel soft materials with unprecedented functions.

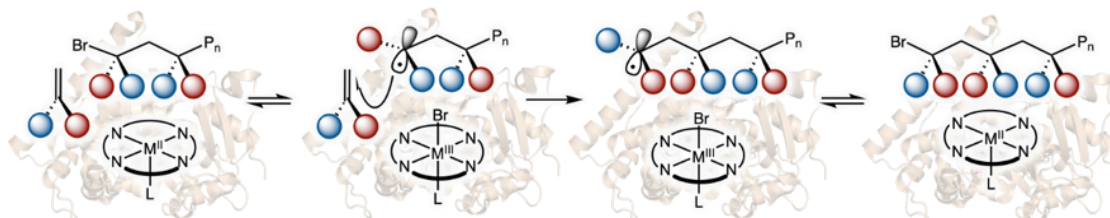


Fig. 23. Engineering heme and cobalamin-dependent proteins for stereocontrolled radical polymerization.

Research Progress: We aim to engineer metalloenzymes to catalyze living radical polymerization in a stereocontrolled fashion and to study the structure-property relationships of novel polymeric materials (**Fig. 23**). Toward this goal, we have accumulated more than 300 variants of diverse Fe, Co and Cu proteins, including Fe enzymes (heme and nonheme enzymes), Co proteins (cobalamin-dependent proteins), and Cu enzymes (e.g., galactose oxidases, tyrosinases and laccases). This in-house metalloprotein library will serve as the basis for the development of new-to-nature metalloredox biocatalytic processes.

We evaluated our Fe enzyme collection and identified initial hits in several enzyme families. In the heme protein family, several protein variants including P450s (40–1000 TTN, TTN = total turnover number), globins (30–40 TTN) and cytochromes *c* (20–30 TTN) were found to promote this unnatural reaction. In the nonheme enzyme family, an α -ketoglutarate (α -KG)-dependent ethylene forming enzyme (*PsEFE*) bearing a His-His-Glu facial triad (30 TTN) and a sulfoxide synthase (*EgtB*) involved in ergothioneine biosynthesis bearing a His-His-His facial triad (20 TTN) also facilitated this process. Several Cu-dependent enzymes (e.g., *Tm* laccase) also showed initial activity. Due to their higher enantioselectivities, our initial directed evolution focused on P450 enzyme variants derived from CYP102A1. Five rounds of site-saturation mutagenesis (SSM) by targeting active-site residues and screening led to a new metalloenzyme P450^{ATRAse1}, furnishing the enantioenriched lactam product in 97% yield, 97:3 enantiomeric ratio (e.r.) and 20,000 TTN. Kinetic characterization of this evolved P450^{ATRAse} showed a turnover frequency (TOF) of 24,000 h⁻¹. The kinetics of this evolved enzyme approaches those of natural enzymes, thus demonstrating the excellent activity of these laboratory-evolved biocatalysts. These efforts set the stage for further study on atom transfer radical polymerization.

Future Plans: We have begun to investigate ATRP using some of the metalloproteins we studied in our model ATRC systems. Further work in the next stage of research (year 2) will afford ATRPases with enhanced control, ultimately leading to polymeric materials with unique properties.

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Seeds

iSuperSeed

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Selecting for Phase-Separating Nucleic Acid Coacervates

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Electronic Structure and Scattering Mechanisms in Twisted Bilayer Graphene

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6. EDUCATION AND HUMAN RESOURCES

UCSB MRSEC education staff and researchers are dedicated to improving access to science for diverse groups and to building a competent work force of scientists and engineers. Our education programs provide undergraduate research opportunities, graduate student training, outreach to K-12 students and teachers, and community outreach.

UCSB MRSEC Undergraduate Research Programs

UCSB MRSEC Education Programs currently run six undergraduate research intern programs including Research Interns in Science and Engineering (RISE), Future Leaders in Advanced Materials (FLAM), UCSB PREM with Jackson State University, UCSB PREM with University of Texas at El Paso, California Alliance for Minority Participation (CAMP) and Cooperative International Science and Engineering Internships (CISEI). Our longtime strategy has been to leverage funding from other NSF awards in order to better serve our stakeholders; CAMP and PREM are fully funded from other NSF awards, CISEI is partially funded by an NSF IRES grant, while RISE and FLAM are primarily funded by the MRSEC. In 2021, due to COVID-19 restrictions, all of our undergraduate research programs were affected; FLAM, PREM and CAMP were run in hybrid fashion, with some students participating in-person, some remotely, and some who were able to move from remote to in-person at some point during the summer. All were reduced in size due to the difficulty in placing students as the campus was starting to accept undergraduates back into labs. CISEI, which sends students overseas, went on hiatus for a second summer. Here we report on the outcomes of students who were funded in part or wholly by the MRSEC (including UTEP and JSU PREM which are run concurrently with FLAM).

The UCSB MRSEC FLAM program supports research experiences for undergraduate students in science and engineering during the summer at UCSB. The RISE program supports school year internships for UCSB students. FLAM and RISE students are placed in research laboratories and assigned an individual mentor, usually a graduate student or postdoctoral researcher. Students also participate in weekly intern group meetings, practice giving oral presentations on their research, and produce final written and oral reports. Students in the summer 2021 program also attended a weekly Zoom career building workshops, including Tips on Talks, Figures for Presentations, Poster Making, Finding Positions in Industry, Graduate School Panel, and others. The workshop information was shared with other program coordinators and the sessions were regularly attended by participants from other intern programs at UCSB. All FLAM interns participated in an in-person Summer Undergraduate Research Colloquium at the end of the summer.

Summer 2021 FLAM ran from June 21 to August 20, 2021. 15 students participated fully in the FLAM program, of which 12 were funded at least partially by the MRSEC. In addition to center funding, FLAM also leveraged funding from the UCSB College of Engineering and the UCSB UTEP PREM. Students were recruited nationally and selected with a particular focus on women, underrepresented minority students, first generation college-goers, and students from non-PhD granting and other non-UCSB colleges and universities. In summer 2021 a particular emphasis was placed on students from California colleges and universities due to the difficulties in travel and group housing. The participating interns came from 6 different colleges and universities. In this cycle we supported 22 UCSB undergraduate research interns through the school-year RISE program. Interns were included on 14 refereed publications in this cycle (listed below). FLAM, PREM and RISE research project information can be found on the Center website. Demographics for the summer FLAM program are provided on the next page:

Summer FLAM Interns 2021 (includes PREM)	No. of Interns	Percent of Total
Total	15	100%
Female	10	67%
URM	5	33%
1 st generation college	3	20%
Non-PhD granting Inst	5	33%
Non-UCSB students	7	47%

Undergraduate Career Development Programs

As part of our continued effort to provide career development and support for undergraduates at UCSB, we have initiated a variety of professional development seminars and workshops that we present throughout the year:

Activity	Terms	# MRSEC Participants
Applying for Internships	Fall, Winter	40
Resources for Undergraduate Success Workshop	Winter	9
Python Bootcamp	Summer	25
Graduate Student Panel and Workshop	Summer	25
Careers in Industry Workshop	Summer	25
LinkedIn Workshop	Summer	25
Figures for Presentations Workshop	Summer	25
Tips on Talks Workshop	Summer	25
Poster Presentation Workshop	Summer	25
Writing an Abstract Workshop	Summer	25
Oral Presentation Workshop	Summer	25
Poster Colloquium	Summer	25

UCSB MRSEC Teacher Programs

Research Experience for Teachers (RET). The UCSB MRSEC RET program is designed to immerse local secondary science teachers in the research environment and to support their efforts to create innovative science curricula. Summer 2021 marked the program's twenty-third year. The RET program is a 2-summer commitment. The first year, teacher participants work in a research laboratory with a mentor for six weeks. They attend weekly group meetings where they share details of their research through structured presentations. They also attend the weekly summer seminars and do a final oral presentation on their projects, an event to which their mentors are also invited. During the school year after the research experience, program staff meet with the teachers at least twice to guide them in considering how some aspect of their research experiences can be integrated into their instructional programs. During a second summer, the teachers return to UCSB for four weeks in order to design lessons or units reflecting this instructional integration. They then test their lessons during the subsequent school year. The culminating event for the RET teachers is an annual March workshop in which they present their projects to secondary teachers from the tri-county area. This workshop has also been an effective mechanism for recruiting new

teachers for the next summer's cohort. Teachers are recruited from middle and high schools in Santa Barbara, Ventura and Los Angeles Counties. Preference is given to teachers from low-performing schools and those without prior research experience.

During Summer 2021, the RET program moved to hybrid programming. Three RET I teachers were funded by the UCSB MRSEC and conducted remote research projects. Two teachers developed lesson plans under RET II and will present them remotely for the 2022 UCSB MRSEC Secondary Curriculum Workshop to be held on April 30, 2022. All RET lesson plans and curriculum materials are available online on the UCSB MRSEC website (<http://www.mrl.ucsb.edu/RET>). As of March 2022, 82 curriculum projects are archived.

Informal K–12 Education Programs

UCSB ScienceLine. ScienceLine is an internet-based question and answer service that connects UCSB MRSEC researchers with K–12 schools. Students and teachers submit questions online and receive a response from one or more scientific researchers within a week. All the questions and responses are entered into a searchable online archive, which itself is a useful curriculum supplement for science teachers. In 2021 we received 172 questions bringing the total archived questions and answers to 7153. The ScienceLine website, including the question/answer archive, receives over 8,000 visits per day on average. However, ScienceLine is designed to primarily serve local schools and teachers; in 2021 90 questions came from California schools. In 2021, 205 UCSB scientists, including faculty, postdocs, graduate students, undergraduates and alumni participated by answering questions.

Build your own Buckyball. In 2007 UCSB MRSEC Director **Seshadri** and Education Director **Dorothy Pak** received a Faculty Outreach Grant (FOG) to update and extend our popular presentation centered on a Carbon-60 molecular model kit. UCSB MRSEC Education Staff and graduate students regularly present a Carbon-60 molecular model kit designed to teach K–12 students about nanoscience, chemical bonding and the relationship between structure and properties in materials. In 2021–22 we presented the activity to **102** elementary students in 5 classrooms, assisted by 8 graduate student and post doc volunteers.

Solar Car Workshops. In 2011 UCSB MRSEC Director **Seshadri** and Education Director **Dorothy Pak** received a FOG grant to develop a new hands-on workshop on alternative energy and photovoltaics. In 2021 we presented our modified remote solar car activity over Zoom to **67** elementary and middle school students, assisted by 8 graduate student and post doc volunteers.

Remote Activities. When COVID-19 shut down schools in Santa Barbara County, we actively reached out to support our teacher network through virtual connections to the MRSEC. Teachers expressed their desire for hands-on and inquiry-based activities as well as career pathway discussions with MRSEC graduate students. In response, MRSEC graduate students and faculty offered a variety of new remote activities including 'The Materials Science of Chocolate', 'Hydrophobic materials', 'Materials Science of Slime', 'Investigating the Acoustic Levitator', 'Modeling Cartilage', and the 'Photoelastic Effect'. In 2021–22, although classrooms returned to in-person education, field trips and guest lecturers were severely limited; we presented remote activities to **905** junior high school students in 33 different classes. The majority of these (23 classrooms, 785 students) were junior high school classes in the high minority serving Oxnard School District. Graduate students presenting these activities have also produced 2-minute videos of themselves in the laboratory, so that they could give students a virtual lab tour and facilitate discussion of career pathways.

Education Program REU and RET Projects, March 2021–February 2022*REU Projects Summer 2021*

Hollingshaus, Gunnar, Materials Engineering, California Polytechnic State University, San Luis Obispo, Sam Daly, Caelin Muir, “Comparison of Machine Learning Frameworks for Acoustic Emissions of SiC/SiC Composites”.

Marquez, Emily, Chemistry, California State University, Long Beach, Yang Yang, Michael Chin, “Directed Evolution of Metalloenzymes for Stereo-controlled Atom Transfer Radical Addition and Polymerization”.

Soto, Maria, Chemical Engineering, California State University, Long Beach, Chris Bates, Chungryong Choi, “Degradable Elastomers Based on Sustainable and Green Chemistry”.

Goudreau, Meredith, Chemistry, Las Positas College, Ram Seshadri, Emily Morgan, “Solid-State Synthesis and Density Functional Theory Investigation of Mo-Based Vacancy Ordered Double Perovskites”.

Taddese, Eden, Chemical Engineering, University of Kansas, Craig Hawker, Lindsay Robinson, “Investigating the Effect of Dynamic Covalent Boronate Crosslinks on the Interlayer Strength of 3D-Printed Networks”.

Bae, Rachel, Chemistry, UCSB, Angela Pitenis, Johan Rosas, “Modeling Tissue Mechanics with Packed Granular Hydrogel Assemblies”.

Jasuja, Dev, Physics CCS, UCSB, Paul Atzberger, “Exponential Integrators for Simulating Stochastic Dynamical Systems”.

Jin, Wen, Chemical Engineering, UCSB, Raphael Clement, Emily Foley, “Manganese- and Iron-based Weberites as High Energy Density Na-ion Battery Cathode Materials”.

Deglurkar, Shivani, Mechanical Engineering, UCSB, Elliot Hawkes, Nicholas Naclerio, “Exploring Light-Sensitive Materials for a Self-Steering Vine Robot”.

Romero, Rebecca, Material Science and Engineering, University of Texas at El Paso, Irene Beyerlein, Shouzhi Xu, “Atomistic calculations of the generalized stacking fault energies and local slip resistances in three refractory multi-principal element alloys”.

Bear, Soren, Physics, UCSB, Stephen Wilson, Ganesh Pokharel, “Effect of Lu-doping on magnetic ordering in the quantum spin liquid candidate NaYbSe₂”.

Asham, Kareem, Chemistry and Biochemistry, California State University, Long Beach, Rachel Segalman, Gordon Pace, “Design and Analysis of Mixed Ion and Electron Conducting Polymers”.

Carrel, Gabrielle, Physics, UCSB, Ram Seshadri, Aurland Hay, “Prediction and Synthesis of Potential Topological Superconductors”.

Shandu, Shaan, Electrical Engineering, UCSB, Upamanyu Madhow, Lalitha Giridhar and Maryam Eslami Rasekh, “Measuring MIMO Channel Robustness Through Alterations in Receive Antenna Alignment”.

Lewis, Erin, Chemistry and Biochemistry, UCSB, Carlos Levi, Tom Drtina, "Thermochemical Compatibility of $\text{HfO}_2\text{-YbO}_{1.5}$ and $\text{ZrO}_2\text{-YbO}_{1.5}\text{-LaO}_{1.5}$ with $\text{AlO}_{1.5}$ ".

RISE School Year Participants Spring 2021, Fall 2021 and Winter 2022

Gans, Ruby, Mechanical Engineering and Physics, UCSB, Paolo Luzzatto-Fegiz, "Spatially Developing Canopy Flow Modeling".

Choi, Dylan, Chemistry, UCSB, Quyen Nguyen, Nora Schopp, "Machine Learning in Organic Photovoltaics".

Wu, Claire, Chemical Engineering, UCSB, Michael Chabiny, Veronica Reynolds, "Predicting Energy-Dependent X-Ray Scattering through Simulated Polymer Morphologies".

Zaveri, Aryan, Physics, UCSB, Raphael Clement, Eliovardo Gonzalez-Correa, "Predicting ssNMR shifts through DFT Simulations on NASICON- $\text{Na}_{3+x}\text{V}_2\text{-xMg}_x(\text{PO}_4)_3$ Cathode for Na-Ion Batteries".

Bear, Soren, Physics, UCSB, Stephen Wilson, Ganesh Pokharel, "Analysis of Magnetoentropic Data for RV_6Sn_6 ".

Perkins, Ryan, Mechanical Engineering, UCSB, Frank Kinnaman, "Silicone 3D Printer".

Wolczko, Sophia, Physics, UCSB, Vojtech Vlcek, Gwen Weng, "Thermally-driven changes in lattice-NV center interaction in the electronic structure of diamond".

Man, Steven, Mechanical Engineering, UCSB, Frank Kinnaman, "Silicone 3D Printer".

Devata, Abhiram, Chemical Engineering, UCSB, Michael Gordon, Pavel Shapturenka, "Computational Study of High Contrast Gratings for Deep UV Light Reflectors".

Kreymborg, Paul, Physics, UCSB, Zvonimir Dogic, Ray Adkins, "Tracking filaments in active nematics".

Jin, Wen, Chemical Engineering, UCSB, Raphael Clement, Emily Foley, "Manganese- and Iron-based Weberites as High Energy Density Na-ion Battery Cathode Materials".

Kwon, Andrew, Chemical Engineering, UCSB, Raphael Clement, Vincent Wu, "Tuning Electrochemical Performance of Allumidite Compounds for Na-ion Battery Cathodes".

Mitra, Ritika, Chemical Engineering, UCSB, Michael Gordon, Pavel Shapturenka, "Computationally investigating light extraction in hole array, reflector-integrated LED structures".

Gutierrez, Juan, Biological Sciences, UCSB, Cyrus Safinya, Christine Tchouwnou, "The Effect of Site-Specific Tau Mutations on Microtubule Bundle Structures".

Lopez, Diego, Chemical Engineering, UCSB, Michael Gordon, Oleksandr Polanskyi, "Surface patterning and wettability control of polymers, using organized streamer patterns in DBD plasmas".

Ladabaum, Max, Physics, UCSB, Andrew Jayich, Craig Holliman, "Laser Cooling of 225Ra^+ ".

Yee, Elexa, Biochemistry, UCSB, Herb Waite, “An investigation of how coacervates insulate mussel foot proteins from oxidation”.

Gebretsadkan, Samuel, CCS Physics, UCSB, Andrew Jayich, Minyu Fan, “Measuring the D5/2 state quadrupole moment of Radium-225+”.

Jobanputra, Anjali, Pharmacology, UCSB, Cyrus Safinya, Christine Tchouwnou, “The Effect of Site-Specific Tau Mutations on Microtubule Bundle Structures”.

Wei, Jason, Mechanical Engineering, UCSB, Frank Kinnaman, “Silicone 3D Printer”.

Krohn-Hansen, Benjamin, Biochemistry, UCSB, Yang Yang, Natalia Neris, “Engineering enzymes for novel radical polymerization reactions”.

Wang, Yijing, Chemical Engineering, UCSB, Matthew Helgeson, Chelsea Edwards, “The influence of mixing methods and component ratios on the formation of complex microstructure of polyelectrolyte coacervate”.

Woodhouse, Kegan, Mechanical Engineering, UCSB, Samantha Daly, Andrew Christison, “Understanding Processing Effects on the Superelastic Behavior of Nitinol”.

RET 1 & 2 2021

Barbara Weiser Santa Paula High School

Mentor: Emily Lau PI: Todd Oakley, There's a thin line between attraction and repulsion: Understanding intermolecular forces with TLC

Cindy Martin Isbell Middle School

PI: Seth Peterson, Estimating crop yields in South Sudan

Tori Pool Bishop Diego High School

Mentor: Louis Graup, PI: Naomi Tague, Combatting Climate Change, from the Microscopic to Macroscopic

Tiffany Cunningham Santa Maria High School

Mentor: Jacob Blankenship PI: Chris Bates, Biodegradable Thermoplastic Elastomers & Supramolecular Dynamic Networks: A Short Study into Polymers

Melissa Wilson Riviera Ridge School

Mentor: Audra Destefano PI: Rachel Segalman, Self Assembly of Polymers

Evaluation and Impact of Education and Outreach Activities

Education program staff members are committed to evaluating our programs to assess their impact and effectiveness. Formative assessment is conducted as part of each program, in the form of participant surveys, interviews, and collection of demographic data. We have also been active in promoting cross-site assessment of MRSEC Education programs, including adoption of the URSSA evaluation instrument for our REU programs.

Since 2018, external evaluator Dr. Ellie Sciaky (UCSB Center for Science and Engineering Partnerships) has conducted an evaluation of the RET program as well as the effects/benefits of teachers' long-term connection to the MRSEC. Efforts include focus groups of current RET teachers and email surveys of past participants. Results indicate a 50% response rate of teacher participants since 1999. 88% of the respondents indicate that RET had a moderate to strong influence on their teaching. Half of all respondents continue to use their own or someone else's RET curriculum project in their classroom; this is a remarkable result since a third of the respondents participated in RET over 10 years ago. The greatest perceived benefit of participation is (79%) building a stronger connection to the scientific research community. Formative assessment of the RET program indicates that placement with an enthusiastic mentor was key to satisfaction with the program.

In addition, we are evaluating the benefits of participating in the MRSEC for graduate students and postdocs. Since fall 2018, Dr. Sciaky has administered an annual survey of 300 UCSB graduate students and postdocs in MRSEC-related fields; results indicate that students with any level of involvement in the MRSEC are more likely to be co-advised than respondents with no involvement in the MRSEC, particularly by faculty in different fields. Students and postdocs who reported any level of involvement in the MRSEC are more likely to participate in opportunities to expand their professional development; Students and postdocs with involvement in the MRSEC are more satisfied with their access to resources; Students with any level of involvement report high satisfaction with their sense of community, particularly those from Materials. Overall, participation in the MRSEC has significant benefits beyond the level of funding that students or postdocs may receive.

Intern Presentations at National Meetings and Awards (Interns in Bold)

Fox Bravo, "Growth and Antibiotic Testing in Sulfate Reducing Bacteria", ABRCMS Conference, Virtual, November 10-13, 2021.

Rebecca Romero, Atomistic Simulations of the Local Slip Resistances in Four Refractory Multi-principal Element Alloys", World Congress of High Entropy Alloys, Charlotte, North Carolina, December 5-8, 2021.

Intern Publications (Interns in Bold)

[1] M. Areyano, J. A. Booth, **D. Brouwer**, L. F. Gockowski, M. T. Valentine, R. M. McMeeking, Suction-controlled detachment of mushroom-shaped adhesive structures, *J. Appl. Mech.* **88** (2021), 031017. DOI: 10.1115/1.4049392

[2] S. W. Baek, K. E. Wyckoff, D. M. Butts, **J. Bienz**, A. Likitchachawankun, M. B. Preefer, M. Frajnkovic, B. S. Dunn, R. Seshadri, L. Pilon, Operando calorimetry informs the origin of rapid rate performance in microwave-prepared TiNb_2O_7 electrodes, *J. Power Sources* **490** (2021), 1–9. DOI: 10.1016/j.jpowsour.2021.229537

[3] N. D. Dolinski, E. B. Callaway, C. S. Sample, L. F. Gockowski, **R. Chavez**, Z. A. Page, F. Eisenreich, S. Hecht, M. T. Valentine, F. W. Zok, C. J. Hawker, Tough multimaterial interfaces through wavelength-selective 3D printing, *ACS Appl. Mater. Interfaces* **13** (2021), 22065–22072. DOI: 10.1021/acsaami.1c06062

- [4] E. Foley, A. Wong, R. C. Vincent, A. Manche, **A. Zaveri**, E. Gonzalez-Correa, G. Menard, R. J. Clement, Probing reaction processes and reversibility in earth-abundant Na_3FeF_6 for Na-ion batteries, *Phys. Chem. Chem. Phys.* **23** (2021), 20052–20064. DOI: 10.1039/d1cp02763h
- [5] S. Ghosh, N. Barman, E. Gonzalez-Correa, M. Mazumder, **A. Zaveri**, R. Giovine, A. Manche, S. K. Pati, R. J. Clement, P. Senguttuvan, Elucidating the impact of Mg substitution on the properties of NASICON- $\text{Na}_{3+y}\text{V}_{2-y}\text{Mg}_y(\text{PO}_4)_3$ cathodes, *Adv. Funct. Mater.* **31** (2021), 2105463. DOI: 10.1002/adfm.202105463
- [6] Y. Kwon, **J. H. Bernstein**, N. Cohen, M. T. Valentine, On-demand manufacturing capabilities of mussels enable robust adhesion to geometrically complex surfaces, *ACS Biomater. Sci. Eng.* **7** (2021), 5099–5106. DOI: 10.1021/acsbmaterials.1c00845
- [7] S. Lantin, **S. Mendell**, G. Akkad, A. N. Cohen, X. Apicella, E. McCoy, E. Beltran-Pardo, M. Waltemathe, P. Srinivasan, P. M. Joshi, J. H. Rothman, P. Lubin, Interstellar space biology via project starlight, *Acta Astronaut.* **190** (2022), 261–272. DOI: 10.1016/j.actaastro.2021.10.009
- [8] P. A. Leggieri, **C. Kerdman-Andrade**, T. S. Lankiewicz, M. T. Valentine, M. A. O'Malley, Non-destructive quantification of anaerobic gut fungi and methanogens in co-culture reveals increased fungal growth rate and changes in metabolic flux relative to mono-culture, *Microb. Cell Fact.* **20** (2021), 2–16. DOI: 10.1186/s12934-021-01684-2
- [9] **R. A. Romero**, S. Xu, W.-R. Jian, I. J. Beyerlein, C.V. Ramana, Atomistic simulations of the local slip resistances in four refractory multi-principal element alloys, *I. J. Plast.* **149** (2022), 103157. DOI: 10.1016/j.ijplas.2021.103157
- [10] E. Sebti, H. A. Evans, H. Chen, P. M. Richardson, **K. M. White**, R. Giovine, K. P. Koirala, Y. Xu, E. Gonzalez-Correa, C. Wang, C. M. Brown, A. K. Cheetham, P. Canepa, R. J. Clement, Stacking faults assist lithium-ion conduction in a halide-based superionic conductor, *J. Am. Chem. Soc.* **144** (2022), 5795–5811. DOI: 10.1021/jacs.1c11335
- [11] N. A. Schauer, **G. A. Kliegle**, P. A. Cooke, R. A. Segalman, R. Seshadri, Database creation, visualization, and statistical learning for polymer Li^+ electrolyte design, *Chem. Mater.* **33** (2021), 4863–4876. DOI: 10.1021/acs.chemmater.0c04767
- [12] **V. J. Shenoy**, C. E. R. Edwards, M. E. Helgeson, M. T. Valentine, Design and characterization of a 3D-printed staggered herringbone mixer, *Biotechniques* **70** (2021), 285–289. DOI: 10.2144/btn-2021-0009
- [13] R. C. Vincent, J.-X. Shen, M. B. Preefer, **J. Lin**, F. Seeler, K. Schierle-Arndt, K. A. Persson, R. Seshadri, Prospects for employing lithium copper phosphates as high-voltage Li-ion cathodes, *J. Phys. Chem. C* **125** (2021), 13123–13130. DOI: 10.1021/acs.jpcc.1c01406
- [14] K. E. Wyckoff, J. L. Kaufman, S. W. Baek, C. Dolle, J. J. Zak, **J. Bienz**, L. Kautzsch, R. C. Vincent, A. Zohar, K. A. See, Y. M. Eggeler, L. Pilon, A. Van der Ven, R. Seshadri, Metal–metal bonding as an electrode design principle in the low-strain cluster compound $\text{LiScMo}_3\text{O}_8$, *J. Am. Chem. Soc.* **144** (2022), 5841–5854. DOI: 10.1021/jacs.1c12070

7. POSTDOCTORAL MENTORING PLAN AND DATA MANAGEMENT PLAN

Postdoctoral Mentoring Plan

The UC Santa Barbara MRSEC takes the mentoring of postdoctoral researchers very seriously, with the aim of helping them reach their career goals, whether those be in academia, National Laboratories, start-ups or established industry. The UC Santa Barbara MRSEC sees the training of graduate students and postdoctoral researchers as part of a continuum, and much of the training and mentoring described below equally applies to both groups. The IRGs and Seed awards explicitly request that postdoctoral fellows are jointly advised and that weekly meetings with both advisors are encouraged. Prior experience has demonstrated that joint advising/mentoring of postdoctoral researchers creates a more productive, fulfilling work environment where researchers feel a shared sense of mission. The different perspectives provided by multiple advisors also gives postdoctoral fellows a leg up in their job searches.

MRSEC postdoctoral fellows are strongly encouraged to network, especially via travel to conferences, symposia, and workshops so that they can connect with the appropriate audiences for advancing their career goals. We provide funds and suggest every MRSEC-supported postdoctoral researcher attend at least one major conference (ACS/APS/MRS/Gordon) every year. The UC Santa Barbara MRSEC has been very successful in using alternate funding sources to award these travel fellowships.

In addition to formal training imparted by UC Santa Barbara faculty on aspects of seeking an academic position, postdoctoral fellows are actively involved in speaking and participating in MRSEC seminars and outreach events. They are also involved in planning events and in choosing/inviting speakers to bring to campus (or, during COVID-19, to invite for Zoom seminars). Opportunities to spend time with faculty candidates as well as visitors from academia, industry and National Labs are strongly encouraged. Such informal contact with established professionals exposes postdoctoral scholars to multiple careers.

To complement these activities, the Education Program supports postdoctoral students by providing them with more formal personal and professional development opportunities. MRSEC faculty annually host several short (90 minutes to 2 hr.) career-building workshops. The value of these workshops is evidenced by the large number of non-MRSEC attendees who usually learn of them by word of mouth or through the UC Santa Barbara Graduate Division. The student organization, Graduate Students for Diversity in Science, plays an important role in the organization and advertising of these activities.

The UC Santa Barbara MRSEC is aware that transitioning into and out of postdoctoral positions is hindered by the situation faced across the world in light of the COVID-19 pandemic. MRSEC faculty and staff are working closely with senior graduate students who may be attempting to transition into postdoctoral positions, as well as postdoctoral fellows attempting to transition into faculty and other kinds of positions, to ensure that they are not unduly stressed. While the near-term prospects were initially thought to be rather dire, in reality, UC Santa Barbara postdocs have still had significant success finding academic positions and industrial jobs despite the pandemic. MRSEC faculty and staff continue to provide extra support and flexibility for postdoctoral scholars during these trying times.

Data Management Plan

MRSEC research principally produces research data in the form of lab notebooks, electronic files, samples, and software. The supported MRSEC investigators are responsible for the storing and archiving of samples, and they will make samples available to others upon request following the usual best practices followed by the University and the broader research community. Collecting, tagging, analyzing, publishing, and archiving the vast quantities and types of materials characterization and research data involves an evolving close collaboration between facility managers, researchers, and PIs. Scientific instrumentation resides on a private network and is connected to file servers that have dual-interfaces to facilitate both on-campus and

off-campus connectivity. Raw data also resides on local file servers and is backed up to different buildings on campus as organized and maintained by the IRGs. File shares have been created for specific projects and IRGs as needed. During COVID-19, the UC Santa Barbara MRSEC has been working closely with all research stakeholders (including users of shared facilities) to better accomplish work-from-home tasks. This includes installing hardware and software that enables the remote operation of instruments in MRSEC shared facilities.

Policies for access and sharing including provisions for appropriate protection of privacy, confidentiality, security, intellectual property, or other rights or requirements: By using the Merritt repository, researchers are given fine-grained control over what data to share and when, and sharing occurs primarily over the internet via Merritt's APIs and web interface. Very large datasets may reside on locally hosted UC Santa Barbara MRSEC servers with persistent URLs. The list of MRSEC supported publications is monitored once a year for researcher data management practices and researchers are notified of best-practices and available resources. The University of California, Santa Barbara retains intellectual property rights to the data and publications involving patentable data may be delayed until a patent application is filed. Raw data resides on storage at the UC Santa Barbara MRSEC and it is ensured that all raw data is stored using open formats rather than proprietary ones that could become difficult to use in future.

Policies and provisions for reuse, redistribution, and the production of derivatives: The goal of all the UC Santa Barbara-MRSEC supported research is to widely disseminate the work, with appropriate acknowledgement of the grant, in archival journals. Following current practice, all publication PDF files are provided to the NSF annually for verification of the contents, including acknowledgements. All UC Santa Barbara MRSEC faculty are strongly encouraged to publish postprints of their research on the University of California repository eScholarship. This entity has already negotiated the copyright issues with all major journals to carry such postings, and having this, in effect enables open access. In addition, the University of California Santa Barbara Library has a program in place known as the Open Access Publishing Fund that pays for journal article processing fees associated with open access in reputable, high-impact journals. After publication, these manuscripts are available free of charge for all readers worldwide.

Plans for archiving data, samples, and other research products, and for preservation of access to them: Samples, as mentioned earlier, are the responsibility of individual investigators, who will preserve them for at least 10 years after the end of the award period, provided there are no issues with chemical and physical stability or other hazards. Raw data stores, IRG file shares, researcher and project file shares will be continually migrated to modern systems as necessary to maintain data integrity. Backup and security are maintained by the UC Santa Barbara MRSEC. Researchers will use an existing tape library for long-term data storage and archiving. Tape archives will be kept for 6 years beyond the end of the grant, though primary data may reside in Merritt for much longer.

8. CENTER DIVERSITY – PROGRESS AND PLANS

(a) Current status and progress since the last reporting period

Over the past year, the UC Santa Barbara MRSEC has been committed to increasing diversity, equity, and inclusion (DEI) across all stakeholders. **Pitenis** has coordinated all Diversity, Equity, and Inclusion (DEI) matters at the level of the MRSEC and has served as a bridge between DEI committees across the MRSEC, Materials Department, College of Engineering, and campus. Separately, the UC Santa Barbara campus appointed a new Interim Vice Chancellor for DEI: Professor Jeffrey Stewart, whose appointment has already positively impacted the campus discourse. The campus also appointed three Associate Vice Chancellors for DEI: Professors Ben Refuerzo, Sharon Tettegah, and Kim Yasuda, who have implemented new DEI-focused programs and workshops. The UC Santa Barbara Chancellor Yang appointed **Pollock** as Interim Dean of the College of Engineering, who has made DEI a top priority. The College of Engineering Associate Dean and Faculty Equity Advisor, Professor Elizabeth Belding (Computer Science), has worked alongside **Pitenis** among other PIs across the College to improve recruitment, retention, and mentoring of underserved groups, particularly at the undergraduate and faculty levels. The College of Letters and Science Associate Dean and Faculty Equity Advisor, **Shea**, also serves in this role. Additionally, all of the MRSEC-associated Departments have DEI committees with members of leadership drawn from MRSEC senior investigators who have been working closely with Vice Chancellor Stewart, Associate Vice Chancellors Refuerzo, Tettegah, and Yasuda, as well as Interim Dean of College of Engineering Pollock and Professors Belding and Shea on developing and implementing strategies to improve DEI.

Our K-12 and RET programs serve school populations that are majority Hispanic, and all of the programs highlighted in the previous section are focused on serving and engaging with our diverse local communities. As a recently designated Hispanic-Serving Institution (as of 2015), we are proud of the number of URM undergraduate students mentored through our MRSEC programs (Total: 104; 49% women, 32% URM), including through our two thriving PREM partnerships with UT El Paso and Jackson State University. Of the 104 undergraduate interns directly supported by the MRSEC, 63% have continued on to graduate school; of these students, 50% are women and 45% are URM. The ongoing success of our PREM partnerships is due to the active participation and exchanges of faculty, postdoctoral fellows, graduate and undergraduate students, with joint publications in preparation. The MRSEC also serves as UC Santa Barbara's central location for the University of California system-wide NSF-LSAMP program for URM scholars.

The MRSEC actively encourages URM interns both from UC Santa Barbara and those participating in our summer internship programs to apply for graduate programs nationwide through professional development and career-building activities. We coordinate with MRSECs across the country to connect research interns from UC Santa Barbara with graduate opportunities across other MRSEC programs. Examples of effective coordination among MRSECs includes hosting recruiting and event booths at national conferences such as SACNAS to showcase MRSEC research, facilities, and career development opportunities to the broader scientific community. The UC Santa Barbara MRSEC actively works to integrate all stakeholders across all levels through MRSEC activities. The annual MROP event highlights an effective means of engaging with students and faculty from our PREM partners.

The UC Santa Barbara MRSEC is committed to broadening participation in STEM among underrepresented groups. The PREM partnerships have enabled increased numbers of graduate students recruited from UT EL Paso and Jackson State University. Increasing the diversity of graduate students and postdoctoral fellows is integral to the mission of the UC Santa Barbara MRSEC. Summer internships,

combined with our PREM partnership programs, have been effective in increasing the number of URM graduate students at UC Santa Barbara. We have also worked closely with the Interim Dean of Graduate Division, Leila Rupp, to support her campus-wide graduate diversity initiatives. These efforts are designed to increase support for students from recruitment, transition to graduate school, matriculation, commencement, and beyond. An example includes the close coordination between MRSEC faculty and UCSB Graduate Division in organizing a virtual booth at the 2021 SACNAS conference. All MRSEC Departments are implementing holistic reviews of graduate admissions thanks to encouragement, resources, and training from Graduate Division. Many departments have removed GRE requirements from graduate applications and implemented rubrics (created by **Beyerlein**) to reduce implicit biases. Chairs and members of Graduate Admissions Committees across the UC Santa Barbara MRSEC Departments have all participated in Implicit Bias and Anti-Racism Training. The student-led UC Santa Barbara Graduate Students for Diversity in Science (GSDS), supported by a Dow Aid-to-Education Grant, has made a positive impact on the campus community by advocating for increasing diversity across all levels to expand the STEM pipeline. The 2021 UC Santa Barbara MRSEC Involvement Survey conducted by Dr. Elizabeth Sciaky and Elise Stankus through the Center for Science and Engineering Partnerships reported that increased MRSEC participation among graduate students and postdoctoral fellows correlated with a stronger sense of community and a preference to work in an environment with regular interactions with individuals from diverse or underrepresented backgrounds.

At the faculty level, MRSEC faculty are actively working to recruit UC Presidential Postdoctoral Fellows, comprising a highly competitive pre-selected pool of diverse faculty candidates. **Han** is leading the Young Scientist Award Lecture in the Department of Chemistry and Biochemistry which offers presentation mentorship to current UC Presidential Postdoctoral Fellows. Preliminary evidence suggests that the holistic review process for faculty applicants has increased the number of URM candidates invited to interview on campus. Other initiatives have been implemented – including the National ChemE Seminar Series coordinated by multiple Chemical Engineering Departments nationwide, with **Segalman** among the leaders – to showcase scholars and future faculty from diverse backgrounds and highlight the diversity of the discipline.

(b) Plans for the next reporting period

The UC Santa Barbara MRSEC will continue to strive towards increasing diversity, equity, and inclusion for all stakeholders, ranging from K-12 programs to the addition of new faculty investigators through Seed programs. At the level of undergraduate and graduate students, we are encouraged by the ongoing progress of the PREM partnerships and their positive impact on the demographics of the graduate student body. At the postdoctoral level, we are continuing to leverage commitments from the UC Santa Barbara Graduate Division to expand diversity, equity, and inclusion in accordance with University policy and California state law.

9. KNOWLEDGE TRANSFER TO INDUSTRY AND OTHER SECTORS

The UC Santa Barbara MRSEC is committed to creating intellectual networks and infrastructure that can benefit workforce preparedness of our students, job creation, industry, and society. Key industry partners of UC Santa Barbara include: (1) the Mitsubishi Chemical Center for Advanced Materials (now over 20 years old and in the process of renewal) led by **Fredrickson** who also coordinates all UCSB MRSEC Industrial Outreach), (2) the Dow Materials Institute at UC Santa Barbara (led by **Hawker**), and (3) the BASF California Research Alliance (CARA). These centers interact with the UC Santa Barbara MRSEC in a number of synergistic ways, and the first two (Mitsubishi and Dow) are co-located with the UC Santa Barbara MRSEC. Examples of the synergies include support for facilities, co-staffing with the MRSEC leading to efficiencies, the provision of graduate fellowships, travel grants, and support to the Graduate Students for Diversity in Science organization. The Complex Fluids Design Consortium (most recent meeting in January 2022)—an Academic–Industry–National Lab partnership that has been in existence for over 15 years—also aligns closely with IRG-2 and IRG-3 research. Amalie Frischknecht of Sandia National Labs is a collaborator in the IRG-2 project and a participant in the CFDC. Annually, our industrial partners meet with UC Santa Barbara MRSEC faculty, graduate students, and postdoctoral researchers at a two-day symposium, the Materials Research Outreach Program (MROP), which was held in January. While originally planned as in-person, the event shifted to being virtual because of the continued impacts of the COVID-19 pandemic (**Figure 23**). This event also involves our PREM partners, illustrating the integration of all stakeholders at every level.

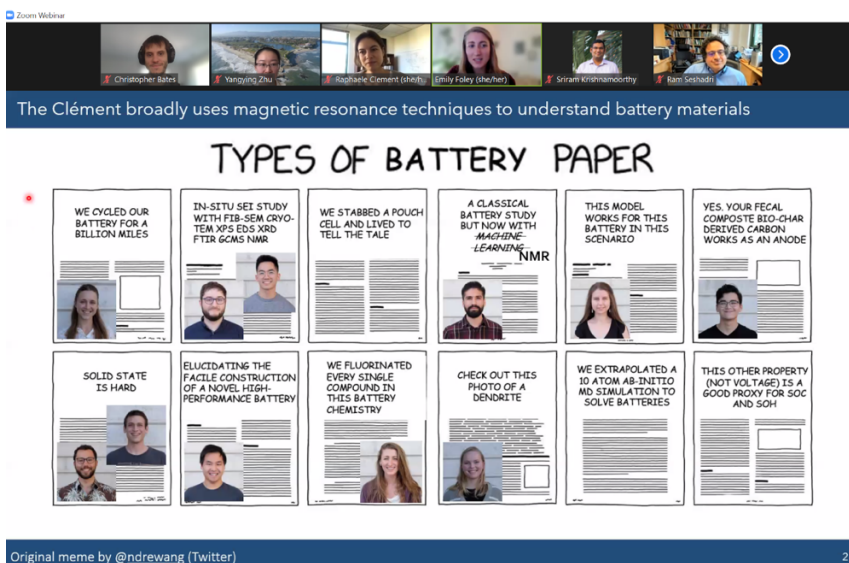


Fig. 23. Graduate student Emily Foley (top center) presenting a Zoom webinar in research in battery materials to an audience of academic, industry, and PREM participants during the 2022 Materials Research Outreach Program.

The combination of fundamental research challenges with an entrepreneurial, multi-disciplinary environment has inspired MRSEC researchers to drive their research beyond traditional boundaries. An example is continued MRSEC support for the annual New Venture Competition (NVC) with the Technology Management Program at UC Santa Barbara which re-envisioned the process of creating start-ups from a faculty-driven model to one led by former graduate students and postdoctoral fellows. Recent MRSEC-supported start-up companies that have won awards at the NVC include Apeel Sciences which is now valued at well over \$1B. A focal point of outreach to industry and to researchers elsewhere are the UC Santa Barbara MRSEC Shared Facilities which, in conjunction with the expertise of the Technical Directors (all Ph.D. scientists), are a unique resource that allows our industrial partners to better understand known materials and design new ones.

10. INTERNATIONAL ACTIVITIES

The UC Santa Barbara MRSEC runs numerous international activities that involve undergraduate and graduate students, postdoctoral fellows, and senior faculty investigators in an integrative and thoughtful manner. The goals are to establish networks and strengthen connections with international IRG affiliates, to leverage research and facilities, and increase the impact of the UC Santa Barbara MRSEC.



Please join us for an international virtual workshop focused on advanced materials for energy and biological applications involving researchers from Chalmers University in Sweden and UCSB. Students, post-docs, researchers, and faculty are all welcome!

All talks will be virtual via Zoom: <https://ucsb.zoom.us/j/83084380979>

Wed 4/28		Program
UCSB Time	Chalmers Time	
9:00-9:10	18:00-18:10	Welcome and Introductions
9:10-9:30	18:10-18:30	Prof. Björn Wickman (Chalmers) Electrocatalyst materials for low temperature fuel cells and electrolyzers
9:30-9:45	18:30-18:45	Student exchange programs
9:45-10:00	18:45-19:00	Emily Foley (UCSB, Clément group) Investigating reaction processes in conversion-type Na ₃ FeF ₆ for Na-ion batteries
10:00-10:15	19:00-19:15	Daise Barbosa de Mattos (Chalmers, Abrahamsson group) Structure-property relationships in chromophore-organogel materials: Consequences for solar energy conversion
10:15-10:30	19:15-19:30	Brian Roehrich (UCSB, Sepunaru group) Impedance Spectroscopy of Single Particles
10:30-10:45	19:30-19:45	Pavel Shapturenka (UCSB, Gordon group) Colloid-based design of bio-inspired structural coloration and optical sensing
10:45-11:00	19:45-20:00	Shun Kondo (Chalmers, Olsson group) Application of scanning TEM to atomic-scale characterization of lattice defects
11:00-11:10	20:00-20:10	Wrap up

Fig. 24. Program for the first of two days, of the Chalmers University-UCSB Virtual Workshop on Advanced Materials for Energy and Biological Applications.

Despite the limitations of interacting with international partners due to the constraints of travel, it was nevertheless an active year for the UC Santa Barbara MRSEC, for such partnerships. We co-hosted a workshop with Chalmers University in Gothenberg, Sweden, one of our several longstanding international partnerships, on April 28th and 29th titled *Advanced Materials for Energy and Biological Applications* (Figure 24). This workshop has spawned continued collaborations and meetings between UC Santa Barbara and international research partners. The workshop included a presentation by Education Director **Pak** on students exchanges between Chalmers and UC Santa Barbara. The restrictions on COVID-19 travel have resulted in undergraduate research exchanges being temporarily curtailed, but the research partnerships between UCSB and Chalmers faculty and graduate students have continued to advance. This has occurred through Zoom meetings and exchanges of samples for measurements and analyses at each institution. With this momentum, we anticipate reciprocal visits, including from students across MRSEC research groups at UCSB, to resume as soon as COVID-19 travel restrictions are lifted.

Also active has been the interaction with scattering groups in France [Aix-Marseille University, and the European Synchrotron Radiation Facility (ESRF) in Grenoble] and as a consequence of joint applications for synchrotron beamtime being successfully competed, MRSEC graduate students will visit the ESRF for experiments in summer 2022.

11. SHARED EXPERIMENTAL AND COMPUTATIONAL FACILITIES

The MRL Shared Facilities have often been referred to as the ‘crown jewels’ of the MRL and indeed they proved their worth during the return to research over the past two years. In terms of finances, the impact of the pandemic on the MRL shared facilities was short-term, with the only dip in recharge income being in the three months that the university was closed. That recovery is due, in large part, to the dedication of all of the shared facilities staff members and their efforts to minimize the impact on researchers during a time of limited access. Staff members made training videos, set up sample drop boxes and remote access, and ran samples as a service, for external users as well as internal. And now, with the benefit of hindsight, the effectiveness of our efforts is clear.

The shared facilities technical staff continue to be active in research, with six co-authored publications collectively in the current grant period. But the Technical Directors, as well as the Faculty Directors are also actively consulting and collaborating with both internal and external researchers. Dr. Rachel Behrens (Polymer) is co-PI on a \$700K grant characterizing depuration of domoic acid, a neurotoxin affecting humans, in California crab populations. The grant supports one fulltime staff person (not part of the shared facilities staff) and partially supports Dr. Behrens. Dr. Youli Li, and the entire Xray team, designed and built a next-generation SAX/WAX system dedicated to the characterization of biomaterials for the new BioPacific Materials Innovation Platform (MIP, DMR 1933487) at UC Santa Barbara. Dr. Amanda Strom (TEMPO) was PI on a \$93K CalTestBed/New Energy Nexus project funding early stage, clean-energy entrepreneurs and pairing them testing facilities in the UC system. And in the Spectroscopy facility, Assistant Prof. Raphaële Clément and Dr. Jerry Hu are actively consulting and developing methods for NMR characterization of battery materials with several external companies. Beyond their role in research, the shared facilities continue to grow in their user base and recharge income, making the MRL MRSEC shared facilities both sustainable and critical to research efforts on campus and in our community.

Shared Facility Statistics March 2021 to February 2022

	Active Internal Users	Active External Users	UCSB Departments	UCSB Groups	External Companies and Institutions	Recharged Hours*
Computation*	375	3	25	152	1	na
Energy	21	1	4	8	1	na
Polymer	86	16	10	32	17	6013
Spectroscopy	103	14	9	27	9	16,161
TEMPO**	146	12	12	39	20	28,061
Xray	152	17	6	36	9	7773
Totals						58,008

*Partnered with the California NanoSystems Institute (CNSI) under the rubric Center for Scientific Computing; **Thermal Electronic/Elemental Magnetic Porosity Optical

Computation: (Directors: Frank Brown, Dr. Paul Weakliem, Nathan Rogers) Through the past year all Center for Scientific Computing cluster users have utilized more than 35 million hours of aggregate CPU time. Researchers associated with MRSEC professors account for more than half of aggregate CPU time. The Computation facility staff meet with researchers and prospective faculty and to direct them to the most appropriate computational resource for their needs. Approximately 30 Zoom meetings were held with graduate students and professors explaining cluster and software usage and best practices. An additional “condo cluster” was added to the CSC’s HPC mix and MRSEC funds will be utilized for compute

nodes for MRSEC researchers. The GPU nodes funded from NSF CC* Award 1925717 are heavily used for computational materials chemistry and a wide variety of machine learning endeavors.

Energy: (Director: Prof. Michael Chabiny; Technical Director: Dr. Rachel Behrens) While no new instrumentation has been acquired for the Energy facility this past year, our focus was our current research base. To build a more sustainable facility, we have implemented a nominal daily lab fee. This fee assists in keeping consumables available for the glovebox, Karl Fischer titrator, and potentiostats, in addition to having funds available for emergency repairs.

Polymer: (Director: Prof. Christopher Bates; Lab Manager: Dr. Rachel Behrens) Continuing efforts to expand the Polymer Lab's capabilities have included an upgrade of one of the aging GPC systems. In addition, facility staff consulted with many companies on data interpretation, guidance on instrument purchases and method development. Several on-campus groups have begun collaborations with the Polymer facility staff to take a multi-faceted approach on elucidating additional information from their samples. A two-year grant project, entitled *Identifying missing links in the transfer and retention of domoic acid in commercially important California crab species*, was started with Dr. Carolyn Culver and 3 additional co-PIs in Marine Sciences, utilizing the facility's LC-MS.

Spectroscopy: (Director: Prof. Raphaële Clément; Technical Director: Dr. Jerry Hu) **Spectroscopy:** A 1.3mm single-channel broadband (X-BB) magic-angle spinning (MAS) probe for solid-state NMR was built in-house by the facility staff for the custom 100MHz WB spectrometer. The probe is tunable over a wide frequency range from ^{13}C to ^1H , and covers other technologically important nuclei, such as ^7Li , ^{19}F , ^{23}Na , and ^{31}P , facilitating multi-nuclear NMR experiments on a single sample without opening the probe for tuning. Currently, this probe is the only one dedicated to the 100MHz spectrometer because there are no commercially available NMR probes that can tune to these low frequencies.

TEMPO: (Faculty Director: Prof. Ram Seshadri; Technical Director: Dr. Amanda Strom) The TEMPO facility's most recent equipment addition is the Agilent 5800 ICP-OES for elemental analysis. The 5800 represents the latest in trace-analysis technology and replaces a 15-year-old system, allowing researchers to get more accurate data in much less time. The TEMPO Low Temperature Characterization facility continues to expand our capabilities to the point that we now must also expand staff support. TEMPO will share a fulltime staff person with the Quantum Foundry (DMR 1906325) to focus on application support for our users as well as developing new techniques.

Xray: (Director: Prof. Cyrus Safinya, Technical Director: Dr. Youli Li) During the current period, the x-ray facility launched an effort to convert and upgrade an aging powder diffractometer with a 8 keV Cu x-ray source to an instrument with Mo radiation (17.4 keV) with a solid state linear pixel array detector (Dectris Mythen 21K). This upgrade will provide a high-performance powder XRD with Mo radiation, which has several advantages. Most significantly, it will enhance the in Operando XRD capability of the facility. The upgrade and conversion is being carried out with internal effort including the development of a new instrument control and graphic user interface, an approach designed to provide flexibility to adapt to evolving research needs. The X-ray facility team led the effort to the design and construction of the new advanced SAXS/WAXS instrument in the BioPacific MIP at UCSB, with direct synergistic benefit to x-ray facility users of the MRSEC facilities.

12. ADMINISTRATION AND MANAGEMENT

The current management structure of the UC Santa Barbara MRSEC is displayed below in **Figure 24**. The past year has been the first with the newly changed structure, of the new co-PI and Associate Director, **Bates**, and of **Pitenis** and **Clément** added to the Executive, respectively replacing **Jayich**, **Read de Alaniz**, and **Shea**. The new members has quickly adapted and have provided great leadership. **Hawker**, **Fredrickson**, and **Pak** are the other senior investigators who comprise the overall leadership team, with responsibilities as listed.

The relationships between the main components of the UC Santa Barbara MRSEC — IRG and Seed research, the SEFs, and Education and Outreach — are indicated, along with the specific leadership and advisory structure. The Executive Committee is an internal body comprising IRG Co-Leaders and all of the individuals listed in the organizational chart. The External Advisory Board comprises eight members: Professors Nitash Balsara (UC Berkeley/LBNL), Dan Frisbie (Minnesota), Ka Yee Lee (Chicago), Heather Maynard (UCLA), Stuart Rowan (Chicago), Pat Woodward (Ohio State), and Dr. Michelle Johannes (Naval Research Lab). Professor Ka Yee Lee is no longer continuing on the EAB due to her new duties as Provost at the University of Chicago.

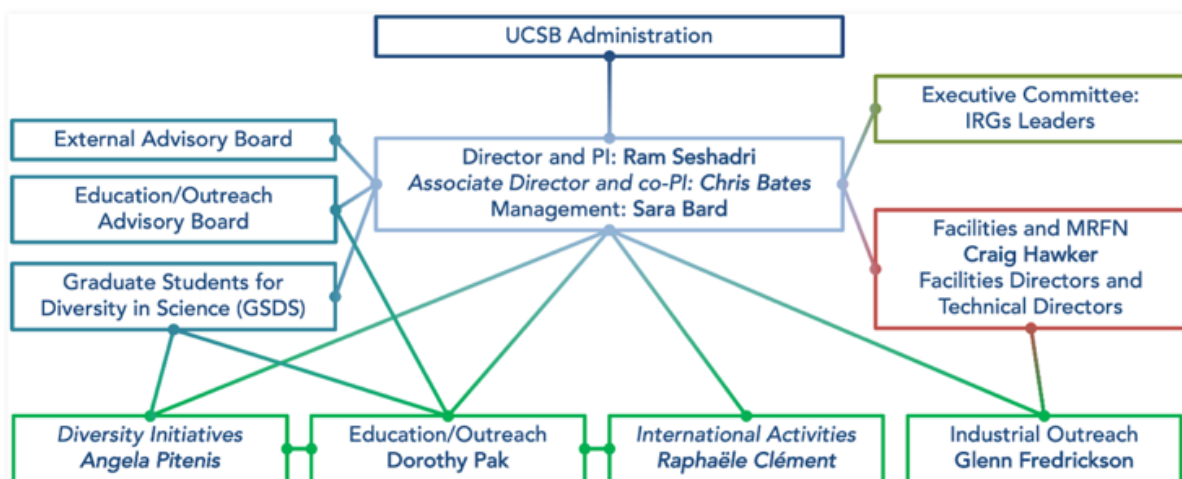


Figure 24: Management structure of the UC Santa Barbara MRSEC. In *italics* are names of faculty PIs who have been brought in recent years to replace others. GSDS is a student-run organization with a focus on expanding diversity, and also serves as the student body advising the UC Santa Barbara MRSEC leadership.

The IRGs are individually managed by the Co-Leaders. All individual IRGs meet once every week. The IRGs carry out internal reviews initially, and then annually to assess progress and to determine funding distribution within an IRG. Senior investigators propose joint advising of graduate students and postdoctoral fellows to be supported by the IRGs, and all decisions are made by the IRG leaders, with help from the Director and Associate Director, and advised by the EAB. The IRGs are not fixed entities, and all three IRGs have transitioned out original members into affiliate status and added new members. The Materials Research Outreach Program (MROP) held in late January 2022 serves as the annual meeting of the entire MRSEC.

The Education and Outreach Program is led by Dr. Dorothy Pak with a team of four part-time coordinators, summing to about 2.5 staff. The team meets on a weekly basis to discuss plans, activities, and program assessment. Evaluator Dr. Elizabeth Sciaky meets with Pak on a quarterly basis.

13. PLACEMENTS: STUDENTS AND POSTDOCTORAL SCHOLARS**GRADUATE STUDENT PLACEMENTS**

Allison Abdilla*	PhD	Staff Scientist, Dow Chemical Corporation
Marcela Areyano* **	PhD	Placement pending
Mitchell Bordelon	PhD	Postdoctoral Researcher, Materials Physics and Applications – Quantum, Los Alamos National Laboratory
Megan Cavanaugh*	MS	Staff Scientist, Clorox
George Degen	PhD	Postdoctoral Fellow, Department of Biological Engineering, Massachusetts Institute of Technology
Rubayn Goh	PhD	Staff Scientist, Institute of Materials Research and Engineering (IMRE), Singapore
Dariya Ignatenko*	MS	Research Associate, EVERY™
Alexander Lill	PhD	Hardware Engineer, PRO Unlimited
Tuan Nguyen	PhD	Senior Process Engineer, C3Nano, Inc. (This is an update. Job placement was reported as unknown in 2020 report.)
Dakota Rawlings	PhD	Independent Consultant
Veronica Reynolds*	PhD	Data Engineer, Citrine Informatics
Manuel Sanchez Zayas**	PhD	Research and Development Scientist, Ph.D. Leadership Development Program, BASF
Jeffrey Self	PhD	Postdoctoral Researcher, Chemical Engineering and Materials Science, University of Minnesota
Marec Serlin	PhD	Placement pending
Tarnuma Tabassum*	PhD	Research Chemist, PPG
William Wonderly	PhD	Placement pending

POSTDOCTORAL SCHOLAR PLACEMENTS

Lianyang Dong	Application Engineer, KLA
Daniil Kitchaev	Research Engineer, Bosch
Hui Nie*	Assistant Professor, Huazhong University of Science and Technology, China
Peter Richardson	Senior Research Scientist, Centre for Process Innovation (CPI), England
Rajarshi Sengupta	Process Development Scientist, Amgen
Philipp Selter	Senior Scientist, Janssen Pharmaceutical Companies of Johnson & Johnson
Jungho Shin	Assistant Professor, Gangneung-Wonju National University, South Korea
Renxuan Xie	Assistant Professor, School for Engineering of Matter, Transport and Energy, Arizona State University
Fulin Wang	Assistant Professor, Department of Materials Science and Engineering, Shanghai Jiao Tong University

* Female

** Underrepresented Minority

14A. LIST OF MRSEC-SUPPORTED PUBLICATIONS

2021-2022 [241]

March 1, 2021 – February 28, 2022

IRG-1 [5]

a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [2]

1. A.L. Beyerlein, I.J. Beyerlein, Bessel function descriptions of magneto-chiral interactions (DMI)-magnetic and spin flexoelectric skyrmions, *Physica B: Condensed Matter* **613** (2021) 412980. DOI: 10.1016/j.physb.2021.412980
2. D.A. Kitchaev, A. **Van der Ven**, Tuning magnetic antiskyrmion stability in tetragonal inverse Heusler alloys, *Phys. Rev. Mater.* **5** (2021) 124408. DOI: 10.1103/PhysRevMaterials.5.124408

b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [3]

3. E. McCalla, E.E. Levin, J.E. Douglas, J.G. Barker, M. Frontzek, W. Tian, R.M. Fernandes, R. **Seshadri**, C. Leighton, Understanding magnetic phase coexistence in $\text{Ru}_2\text{Mn}_{1-x}\text{Fe}_x\text{Sn}$ Heusler alloys: A neutron scattering, thermodynamic, and phenomenological analysis, *Phys. Rev. Mater.* **5** (2021) 064417. DOI: 10.1103/PhysRevMaterials.5.064417
4. P.F. Rottmann, A.T. Polonsky, T. Francis, M.G. Emigh, M. Krispin, G. Rieger, M.P. Echlin, C.G. Levi, T.M. **Pollock**, TriBeam tomography and microstructure evolution in additively manufactured Alnico magnets, *Mater. Today* **49** (2021) 23–34. DOI: 10.1016/j.mattod.2021.05.00323
5. J.L. Zuo, D. Kitchaev, E.C. Schueller, J.D. Bocarsly, R. **Seshadri**, A. **Van der Ven**, S.D. **Wilson**, Magnetoentropic mapping and computational modeling of cycloids and skyrmions in the lacunar spinels GaV_4S_8 and GaV_4Se_8 , *Phys. Rev. Mater.* **5** (2021) 54410. DOI: 10.1103/PhysRevMaterials.5.054410

IRG-2 [10]

a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [7]

6. D.J. Grzetic, K.T. Delaney, G.H. **Fredrickson**, Electrostatic manipulation of phase behavior in immiscible charged polymer blends, *Macromolecules* **54** (2021) 2604–2616. DOI: 10.1021/acs.macromol.1c00095
7. S.K. Jain, D. Rawlings, S. Antoine, R.A. **Segalman**, S. Han, Confinement promotes hydrogen bond network formation and Grotthuss proton hopping in ion-conducting block copolymers, *Macromolecules* **55** (2022) 615–622. DOI: 10.1021/acs.macromol.1c01808
8. S.D. Jones, H. Nguyen, P.M. Richardson, Y.-Q. Chen, K.E. Wyckoff, C.J. **Hawker**, R.J. **Clément**, G.H. **Fredrickson**, R.A. **Segalman**, Design of polymeric zwitterionic solid electrolytes with superionic lithium transport, *ACS Cent. Sci.* **8** (2022) 169–175. DOI: 10.1021/acscentsci.1c01260
9. A. Nikolaev, P.M. Richardson, S. Xie, L.C. Llanes, S.D. Jones, O. Nordness, H. Wang, G.C. Bazan, R.A. **Segalman**, R.J. **Clément**, J. **Read de Alaniz**, Role of electron-deficient imidazoles in ion

- transport and conductivity in solid-state polymer electrolytes, *Macromolecules* **55** (2022) 971–977. DOI: 10.1021/acs.macromol.1c01979
10. N.S. Schausser, G.A. Kliegle, P. Cooke, R.A. **Segalman**, R. **Seshadri**, Database creation, visualization, and statistical learning for polymer Li⁺-electrolyte design, *Chem. Mater.* **33** (2021) 4863–4876. DOI: 10.1021/acs.chemmater.0c04767
 11. N.S. Schausser, P.M. Richardson, A. Nikolaev, P. Cooke, G.A. Kliegle, E.M. Susca, K. Johnson, H. Wang, J. **Read de Alaniz**, R. **Clément**, R.A. **Segalman**, Optimum in ligand density for conductivity in polymer electrolytes, *Mol. Syst. Des. Eng.* **6** (2021) 1025–1038. DOI: 10.1039/D1ME00089F
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b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [3]

13. A. Abdilla, C.A. D'Ambra, Z. Geng, J.J. Shin, M. Czuczola, D.J. Goldfeld, S. Biswas, J.M. Mecca, S. Swier, T.D. Bekemeier, D.S. Laitar, M.W. Bates, C.M. **Bates**, C.J. **Hawker**, Silicone-based polymer blends: Enhancing properties through compatibilization, *J. Polym. Sci.* **59** (2021) 2114–2128. DOI: 10.1002/pol.20210453
14. H. Li, Y. Zhang, S. Jones, R. **Segalman**, G.G. Warr, R. Atkin, Interfacial nanostructure and friction of a polymeric ionic liquid-ionic liquid mixture as a function of potential at Au(1 1 1) electrode interface, *J. Colloid Interface Sci.* **606**, Part 2 (2022) 1170–1178. DOI: 10.1016/j.jcis.2021.08.067
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IRG-3 [23]

a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [8]

16. M. Areyano, J.A. Booth, D. Brouwer, L.F. Gockowski, M.T. **Valentine**, R.M. **McMeeking**, Suction-controlled detachment of mushroom-shaped adhesive structures, *J. Appl. Mech.* **88** (2021) 031017. DOI: 10.1115/1.4049392
17. A.L. Chau, M.K. Cavanaugh, Y.-T. Chen, A.A. **Pitenis**, A simple contact mechanics model for highly strained aqueous surface gels, *Exp. Mech.* **61** (2021) 699–703. DOI: 10.1007/s11340-021-00699-5
18. A.L. Chau, J.M. Urueña, A.A. **Pitenis**, Load-independent hydrogel friction, *Biotribology* **26** (2021) 100183. DOI: 10.1016/j.biotri.2021.100183
19. G.D. Degen, K.C. Cunha, Z.A. Levine, J.H. **Waite**, J-E. **Shea**, Molecular context of dopa influences adhesion of mussel-inspired peptides, *J. Phys. Chem. B* **125** (2021) 9999–10008. DOI: 10.1021/acs.jpcc.1c05218
20. Z. Geng, J.J. Shin, Y. Xi, C.J. **Hawker**, Click chemistry strategies for the accelerated synthesis of functional macromolecules, *J. Polym. Sci.* **59** (2021) 963–1042. DOI: 10.1002/pol.20210126

21. Y. Kwon, J.H. Bernstein, N. Cohen, M.T. **Valentine**, On-demand manufacturing capabilities of mussels enable robust adhesion to geometrically complex surfaces, *ACS Biomater. Sci. & Eng.* **7** (2021) 5099–5106. DOI: 10.1021/acsbomaterials.1c00845
22. V.J. Shenoy, C.E.R. Edwards, M.E. **Helgeson**, M.T. **Valentine**, Design and characterization of a 3D-printed staggered herringbone mixer, *BioTechniques* **70** (2021) 285–289. DOI: 10.2144/btn-2021-0009
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b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [15]

24. M. Ciavarella, G. Cricri, R. **McMeeking**, A comparison of crack propagation theories in viscoelastic materials, *Theor. Appl. Fract. Mech.* **116** (2021) 103113. DOI: 10.1016/j.tafmec.2021.103113
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26. N. Cohen, C.D. Eisenbach, Humidity-driven supercontraction and twist in spider silk, *Phys. Rev. Lett.* **128** (2022) 098101. DOI: 10.1103/PhysRevLett.128.098101
27. V. Deshpande, A. DeSimone, R. **McMeeking**, P. Recho, Chemo-mechanical model of a cell as a stochastic active gel, *J. Mech. Phys. Solids* **151** (2021) 104381. DOI: 10.1016/j.jmps.2021.104381
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32. E.O. McGhee, A.L. Chau, M.C. Cavanaugh, J.G. Rosa, C.L.G. Davidson IV, J. Kim, J.M. Urueña, B.S. Sumerlin, A.A. **Pitenis**, W.G. Sawyer, Amphiphilic gel lubrication and the solvophilic transition, *Biotribology* **26** (2021) 100170. DOI: 10.1016/j.biotri.2021.100170
33. S. Najafi, Y. Lin, A.P. Longhini, X. Zhang, K.T. Delaney, K.S. Kosik, G.H. **Fredrickson**, J.-E. **Shea**, S. Han, Liquid-liquid phase separation of Tau by self and complex coacervation, *Protein Sci.* **30** (2021) 1393–1407. DOI: 10.1002/pro.4101
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PATENTS BY MRSEC-SUPPORTED FACULTY

(a) Patents granted during the current period

Efficient solar cells via sulfur-fused helical perylene diimides design concept

M. **Chabinyk**, F. Wudl, Y. Zheng

U.S. Patent 11,245,077 (02/08/22)

Nanoscale multiple emulsions and nanoparticles

M. **Helgeson**, S. Mitragotri, M. Zhang, M. Nowak, P. Malo de Molina

U.S. Patent 11,254,773 (02/22/22)

(b) Patent applications (excluding provisional applications) during the current period

Design of ligand attachment chemistry for high conductivity polymer electrolytes

R. **Segalman**, A. Nikolaev, C. Sample, J. **Read de Alaniz**, C. **Hawker**, P. Richardson, R. **Clément**

U.S. Patent Application No. 17/191,422 filed 03/03/21

(c) Patents licensed during the current period

Design of ligand attachment chemistry for high conductivity polymer electrolytes

R. **Segalman**, A. Nikolaev, C. Sample, J. **Read de Alaniz**, C. **Hawker**, P. Richardson, R. **Clément**

U.S. Patent Application No. 17/191,422 filed 03/03/21 (licensed 03/03/21)

14.B: INVITED PRESENTATIONS BY MRSEC PRIMARY PARTICIPANTS AT CONFERENCES

1. Chris Bates, "Selective Spin-On Polymer Coatings," 2021 Area Selective Deposition Workshop, March 17, 2021 (virtual). (IRG-3)
2. Chris Bates, "Extreme Mechanical Properties in Elastomeric Materials," Facebook Reality Labs, March 17, 2021 (virtual). (IRG-3)
3. Chris Bates, "Extreme Mechanical Properties in Elastomeric Materials," 3M Non-Tenured Faculty Award Symposium, November 4, 2021 (virtual). (IRG-3)
4. Michael Chabinyk, "Designing Functional Polymers for Organic Electronic Devices," 2021 Materials Research Society Fall Meeting, December 6, 2021 (virtual). (IRG-2)
5. Brad Chmelka, "New mesoporous carbon materials for electrochemical energy conversion applications," Sustainability Seminar Series, Stockholm, March 2, 2021 (virtual). (IRG-3)
6. Brad Chmelka, "Scaling analyses of hyperpolarization transfer from paramagnetic centers into solid media," Global NMR Zoominar, March 9, 2021 (virtual). (IRG-3)
7. Brad Chmelka, "Nanoscale structures and macroscopic properties of platinum-zeolite catalysts," Chevron, April 13, 2021 (virtual). (IRG-3)
8. Samantha Daly, "Machine Learning for High-Throughput Experiment and Analysis of Processing-Property Relationships," Society of Experimental Mechanics (SEM) Annual Conference, June 2021 (virtual). (IRG-1)
9. Samantha Daly, "Machine Learning for the Experimental Mechanics of Structural Materials," Society of Engineering Science (SES) Annual Conference, October 2021 (virtual). (IRG-1)
10. Samantha Daly, "Damage Mechanism Identification in Composites via Machine Learning and Acoustic Emission," BIGMECA International Workshop at SafranTech, November 2021 (virtual). (IRG-1)
11. Zvonimir Dogic, "Active liquid-liquid phase separation," Cornell High Energy Synchrotron Source (CHESS) Workshop, June 10, 2021 (virtual). (iSuperSeed)
12. Zvonimir Dogic, "Active liquid-liquid phase separation," Biological Physics – Physical Biology Seminar, December 10, 2021 (virtual). (iSuperSeed)
13. Glenn Fredrickson, "Field-Theoretic Simulations of Polymers: Bridging Scales and Inverse Design," Australian Society of Rheology, Invited Seminar Series, University of Melbourne, Victoria, Australia, May 17, 2021. (IRG-2)
14. Glenn Fredrickson, "Field-Theoretic Simulations of Polymers and Soft Matter," Nebraska Cluster for Computational Chemistry (NC3) Award Lecture, University of Nebraska, Lincoln, October 15, 2021. (IRG-2)
15. Dan Gianola, "Using Diffraction-Contrast Electron Microscopy to Elucidate Dislocation Pathways in Refractory Multi-Principal Element Alloys," ASM International / Thermo Fisher Scientific Webinar, March 2021 (virtual). (IRG-1)
16. Dan Gianola, "Characterization of defects and their dynamics using transmission scanning electron microscopy," International Conference on Metallurgical Coatings and Thin Films, April 2021 (virtual). (IRG-1)
17. Dan Gianola, "Imaging defects and their dynamics using scanning electron microscopy approaches," Materials Research Society Spring Meeting, April 2021 (virtual). (IRG-1)
18. Dan Gianola, "Imaging defects and their dynamics using scanning electron microscopy approaches," The Minerals, Metals & Materials Society (TMS) Annual Meeting, February 2022, Anaheim, CA. (IRG-1)
19. Craig Hawker, "Faster, Simpler and Better Polymer Synthesis," Australian Polymer Symposium, April 2021. (IRG-3)

20. Craig Hawker, "New Advances in Polymer Synthesis," Pacificchem 2021 Conference, December 2021. (IRG-3)
21. Bolin Liao, "Phonon Transport in Topological Materials," XXIX International Materials Research Congress, August 16, 2021 (virtual). (IRG-1)
22. Bolin Liao, "Thermal Transport in Topological Materials," Materials Research Society Fall Meeting, Boston, MA, December 1, 2021. (IRG-1)
23. Bolin Liao, "Probing Surface Photovoltage Effect Using Photo-assisted Secondary Electron Emission," Pacificchem 2021 Conference, December 17, 2021 (virtual). (IRG-1)
24. Cristina Marchetti, "Kinetic Theory of Defect Dynamics in Active Nematics," American Physical Society (APS) March Meeting, March 2021 (virtual). (iSuperSeed)
25. Cristina Marchetti, "Collective Dynamics of Active Matter," Cargese 2021: Glassy Systems and Interdisciplinary Applications Workshop, July 2021 (virtual). iSuperSeed
26. Angela Pitenis, "Mechanosensing in Monolayer," 10th Annual Southern California Systems Biology Symposium, Beckman Research Institute at City of Hope, Duarte, CA, February 5, 2021. (IRG-3)
27. Angela Pitenis, "Amphiphilic Gel Adhesion," Adhesion Society Conference, San Diego, CA, February 21, 2022. (IRG-3)
28. Tresa Pollock, "Additive Manufacturing of High Temperature Materials: New Alloys and Sustainability Considerations," The Minerals, Metals & Materials Society (TMS) Annual Meeting, March 15, 2021 (virtual). (IRG-3)
29. Javier Read de Alaniz, "Molecules to Devices using Photochromic Dyes," American Chemical Society National Meeting "Breaking Barriers," August 8, 2021 (virtual). (IRG-2)
30. Javier Read de Alaniz, "Molecules to Devices using Photochromic Dyes," 3M, August 8, 2021 (virtual). (IRG-2)
31. Omar Saleh, "A Functional DNA liquid," Materials Research Outreach Symposium (MROP), UCSB, January 26, 2022 (virtual). (Seed)
32. Omar Saleh, "A Functional DNA Liquid," ACS Colloid and Surface Science Symposium, June 14, 2021 (virtual). (Seed)
33. Ram Seshadri, "Designing New Materials with Optimized Functional Properties," Advanced Photon Source Scattering Workshop, Argonne National Lab, October 13, 2021. (IRG-1)
34. Ram Seshadri, "Accelerating the Materials Discovery of Functional Materials," International Workshop on Advanced Materials, Ras Al Khaimah, United Arab Emirates, February 22, 2022. (IRG-1)
35. Joan Shea, "Liquid-Liquid Phase Separation of Proteins," Pacificchem 2021 Conference, December 14, 2021 (virtual). (IRG-3)
36. Megan Valentine, "Nature-inspired materials for load-bearing and actuation," Mechanics of Smart and Tough Gels, International Union of Theoretical and Applied Mechanics (IUTAM) Symposium, May 24, 2021 (virtual). (IRG-3)
37. Vojtech Vlcek, "Stochastic many-body methods for quasiparticle excitations in realistic nanscale systems," American Physical Society March Meeting, March 17, 2021 (virtual). (Seed)
38. Vojtech Vlcek, "Stochastic many-body methods for quasiparticle excitations in realistic nanscale systems," Materials Research Society Meeting, April 22, 2021 (virtual). (Seed)
39. Vojtech Vlcek, "Stochastic many-body methods for quasiparticle excitations in realistic nanscale systems," SIAM Conference on Mathematical Aspects of Materials Science, May 18, 2021 (virtual). (Seed)
40. Vojtech Vlcek, "Stochastic Methods for Many-body Calculations," New Frontiers in Electronic Correlation Conference, June 14, 2021 (virtual). (Seed)

15. BIOS
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PROFESSIONAL PREPARATION

Peking University, China	Chemistry	B.S., 2011
Massachusetts Institute of Technology	Organic Chemistry	Ph.D., 2016
University of California, Berkeley		Postdoc, 2016-2018
California Institute of Technology		Postdoc, 2018 -2020

APPOINTMENTS

2020– Present Assistant Professor, Department of Chemistry & Biochemistry, UCSB
2018 - 2020 NIH Postdoctoral Fellow, California Institute of Technology, Pasadena, California
2016 – 2018 Miller Postdoctoral Fellow, University of California, Berkeley, California

RELEVANT PUBLICATIONS

1. Zhou Q, Chin M, Fu Y, Liu P, Yang Y., Stereodivergent Atom Transfer Radical Cyclization by Engineered Cytochromes P450, *Science* 2021 Dec. 23, 374(6575):1612–1616. PubMed Central PMID: 34941416.
2. Yang Y, Arnold FH. Navigating the Unnatural Reaction Space: Directed Evolution of Heme Proteins for Selective Carbene and Nitrene Transfer. *Acc Chem Res.* 2021 Mar 2;54(5):1209-1225. PubMed Central PMCID: PMC7931446.
3. Yang Y, Cho I, Qi X, Liu P, Arnold FH. An enzymatic platform for the asymmetric amination of primary, secondary and tertiary C(sp³)-H bonds. *Nat Chem.* 2019 Nov;11(11):987-993. PubMed Central PMCID: PMC6998391.
4. Yang Y, Perry IB, Lu G, Liu P, Buchwald SL. Copper-catalyzed asymmetric addition of olefin-derived nucleophiles to ketones. *Science.* 2016 Jul 8;353(6295):144-50. PubMed Central PMCID: PMC5062742.
5. Yang Y, Shi SL, Niu D, Liu P, Buchwald SL. ORGANIC CHEMISTRY. Catalytic asymmetrichydroamination of unactivated internal olefins to aliphatic amines. *Science.* 2015 Jul3;349(6243):62-66. PubMed Central PMCID: PMC4532314.

OTHER SIGNIFICANT PUBLICATIONS:

1. Yang Y, Perry IB, Buchwald SL. Copper-Catalyzed Enantioselective Addition of StyreneDerived Nucleophiles to Imines Enabled by Ligand-Controlled Chemoselective Hydrocupration. *J Am Chem Soc.* 2016 Aug 10;138(31):9787-90. PubMed Central PMCID: PMC5010012.
2. Yang Y. Regio- and Stereospecific 1,3-Allyl Group Transfer Triggered by a Copper-Catalyzed Borylation/ortho-Cyanation Cascade. *Angew Chem Int Ed Engl.* 2016 Jan 4;55(1):345-9. PubMed Central PMCID: PMC4754675.
3. Yang Y, Buchwald SL. Copper-catalyzed regioselective ortho C-H cyanation of vinylarenes. *Angew Chem Int Ed Engl.* 2014 Aug 11;53(33):8677-81. PubMed Central PMCID: PMC4127133.
4. Yang Y, Mustard TJ, Cheong PH, Buchwald SL. Palladium-catalyzed completely linearselective Negishi cross-coupling of allylzinc halides with aryl and vinyl electrophiles. *Angew Chem Int Ed Engl.* 2013 Dec 23;52(52):14098-102. PubMed Central PMCID: PMC3985522.
5. Yang Y, Buchwald SL. Ligand-controlled palladium-catalyzed regiodivergent Suzuki-Miyaura cross-coupling of allylboronates and aryl halides. *J Am Chem Soc.* 2013 Jul 24;135(29):10642-5. PubMed Central PMCID: PMC3776608.

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PROFESSIONAL PREPARATION

Tsinghua University, China	Building Technology	B.S., 2011
Massachusetts Institute of Technology	Mechanical Engineering	Ph.D., 2017
Stanford University	Materials Science	Postdoc, 2017-2019

APPOINTMENTS

2019 – Present Assistant Professor, Department of Mechanical Engineering, UCSB

RELEVANT PUBLICATIONS

- L. Zhao, S. Seshadri, X. Liang, S.J. Bailey, M. Haggmark, M. Gordon, M.E. Helgeson, J. Read de Alaniz, P. Luzzatto-Fegiz, Y. Zhu, "Depinning of Multiphase Fluid Using Light and Photo-Responsive Surfactants", *ACS Central Science*, 10.1021/acscentsci.1c01127.
- Y. Zhu*, J. Xie*, A. Pei, B. Liu, Y. Wu, D. Lin, J. Li, H. Wang, H. Chen, J. Xu, A. Yang, C.-L. Wu, H. Wang, W. Chen, Y. Cui, "Fast lithium growth and short circuit induced by localized-temperature hotspots in lithium batteries", *Nature Communications*, 10, p. 2067, 2019. (*equal contributions).
- H. Wang*, Y. Zhu*, S.C. Kim, A. Pei, Y. Li, D. Boyle, H. Wang, Z. Zhang, Y. Ye, W. Huang, Y. Liu, J. Xu, J. Li, F. Liu, Y. Cui, "Underpotential Lithium Plating on Graphite Anodes Caused by Temperature Heterogeneity", *Proceedings of the National Academy of Sciences*, 117(47), p. 29453-29461, 2020. (*equal contributions).
- Y. Liu, Y. Zhu, Y. Cui, "Challenges and opportunities for fast charging lithium-ion batteries", *Nature Energy*, 4, p. 540-550, 2019.
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- L. Zhao, Y. Qi, P. Luzzatto-Fegiz, Y. Cui, Y. Zhu, "COVID-19: Effects of environmental conditions on the propagation of respiratory droplets", *Nano Letters*, 20(10), p. 7744–7750, 2020.
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- L. Zhang*, Y. Zhu*, Z. Lu, L. Zhao, K.R. Bagnall, S.R. Rao, E.N. Wang, "Characterization of thin film evaporation in micropillar wicks using micro-Raman spectroscopy", *Applied Physics Letters*, 113, p.163701, 2018. doi: 10.1063/1.5048837 (*equal contributions)
- Y. Zhu, D.S. Antao, R. Xiao, E.N. Wang, "Real-Time Manipulation with Magnetically Tunable Structures", *Advanced Materials*, 26(37), p. 6442–6446, 2014. doi: 10.1002/adma.201401515
- H.J. Cho, D.J. Preston, Y. Zhu, E.N. Wang, "Nanoengineered Materials for Liquid-Vapour Phase-Change Heat Transfer", *Nature Reviews Materials*, 2, p. 16092, 2016. doi: 10.1038/natrevmats.2016.92

16. HONORS AND AWARDS

FACULTY

Bates, Christopher

2021, Camille Dreyfus Teacher-Scholar Award
2021, *ACS Polymers Au* Rising Star in Polymers Award

Clement, Raphaele

2022, National Science Foundation Career Award

Daly, Samantha

2021, Fellow of the American Society of Mechanical Engineers (ASME)
2021, American Society of Mechanical Engineers (ASME) Materials Division Centennial Mid-Career Award
2021, Friend of the Committee – US National Committee on Theoretical and Applied Mechanics (USNC/TAM)

Fredrickson, Glenn

2021, Member, National Academy of Sciences
2021, Nebraska Cluster for Computational Chemistry (NC3) Award, University of Nebraska

Liao, Bolin

2021, NASA Early Career Faculty Award
2021, Air Force Office of Scientific Research (AFOSR) Young Investigator Award
2022, Office of Naval Research (ONR) Young Investigator Award

Pitenis, Angela

2021, National Science Foundation Career Award

Pollock, Tresa

2022, Honorary Membership in Société Française de Métallurgie et de Matériaux (SF2M), Paris, France

Van der Ven, Anton

2022, TMS William Hume-Rothery Award, Minerals, Metals & Materials Society (TMS)

Yang, Yang

2021, UCSB Regents' Junior Faculty Award
2022, National Science Foundation Career Award
2022, UCSB Faculty Career Development Award

Young, Andrea

2021, Finalist, Blavatnik National Awards for Young Scientists, New York Academy of Scientists

Zhu, Yangying

2021, Pi Tau Sigma Gold Medal, American Society of Mechanical Engineers (ASME)

GRADUATE STUDENT AND POSTDOC HONORS/AWARDS

Arezano, Marcela

2021, University Award of Distinction, UC Santa Barbara

Chau, Allison

2021, Bright Horizon Global Foundation Materials Department Service Award, UC Santa Barbara
2022, Northern California Society of Tribologists and Lubrication Engineers (STLE) Section Research Scholarship

Degen, George

2021, University Award of Distinction, UCSB
2021, Lindau Nobel Laureate Interdisciplinary Meeting, University of California
Delegate, Lindau, Bavaria, Germany

Getty, Patrick

2021, NSF Graduate Research Fellowship

Luo, Yimin

2021, Otis Williams Postdoctoral Fellowship in Bioengineering, UC Santa Barbara

Plumb, Jayden

2021, U. S. Department of Energy Office of Science Graduate Student Research (SCGSR) fellowship,
Argonne National Laboratory

Vigil, Daniel

2022, Finalist, Padden Award, DPOLY Division, American Chemical Society

17. HIGHLIGHTS

To be presented separately as PowerPoint Files as well as text and image uploads on MRSEC.org

18. STATEMENT OF UNOBLIGATED FUNDS

\$0: All of the funds are fully obligated.