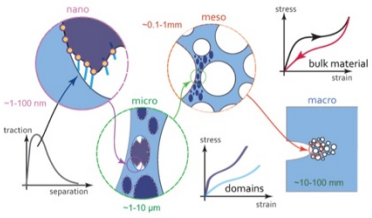
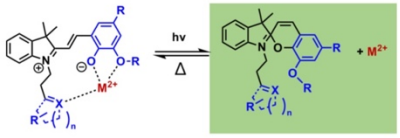
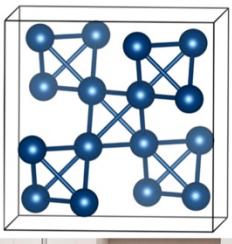
MATERIALS RESEARCH SCIENCE AND ENGINEERING CENTER AT THE UNIVERSITY OF CALIFORNIA SANTA BARBARA

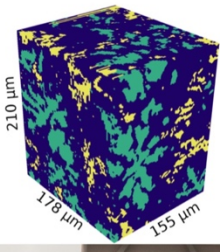
# NSF DMR 1720256 Annual Report

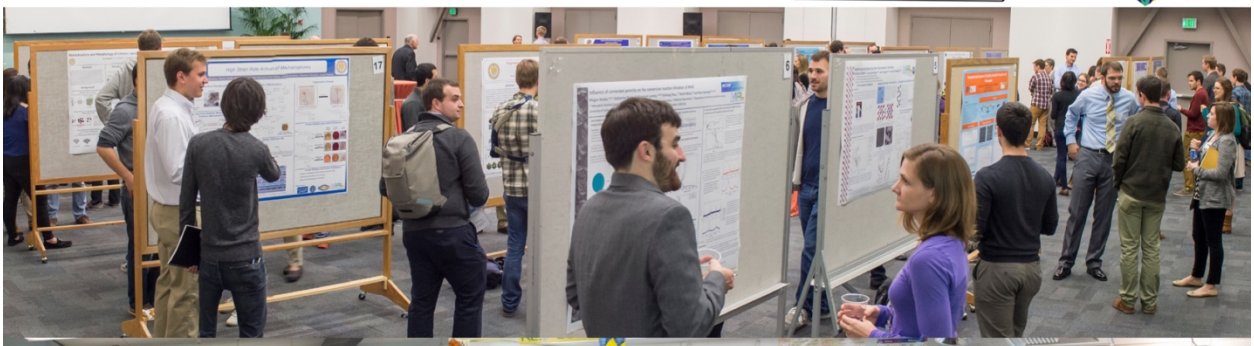
*for the period October 2017 to February 2018*






NSF DMR 1720256

MRSEC

UNIVERSITY OF CALIFORNIA SANTA BARBARA

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# 1. EXECUTIVE SUMMARY

## 1A. Vision and Overview

Materials research is inherently interdisciplinary and major advances require expert input from multiple domains. Materials research is also resource-intensive, and unraveling the details of structure and function to achieve materials-by-design requires development and use of multiple characterization and measurement tools, coupled with high-performance computation. Given these imperatives, the UCSB MRSEC seeks to create the necessary collaborative research and training infrastructure that drives a portfolio of transformative materials research. The UCSB MRSEC aims to be highly inclusive, and involve a broad range of committed participants, with senior investigators drawn from many different departments working collectively toward transformative research outcomes, while nurturing a diverse group of future leaders in materials research. Stakeholders 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, 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 research, Education and Outreach, and Shared Experimental Facilities (SEFs), ensuring that they work in a synergistic and integrative manner.

The vision for UCSB MRSEC success is for it to function organically, as an ecosystem of knowledge-creation and dissemination rather than a site with imposed, top-down management. Students and postdoctoral researchers are encouraged to take leadership roles in education and outreach activities, and they are in turn rewarded by learning to be better teachers and communicators, especially with stakeholders outside of the university research environment. The ethos of collaboration and interdisciplinarity that underpin MRSEC research is also aligned with UCSB traditions.

Current MRSEC Research: The three Interdisciplinary Research Groups (IRGs), all of which are off to a great start as described later on in this report, aim to address vital problems in materials research whose solutions require input from multiple dedicated teams of interdisciplinary researchers. Each of the IRGs will develop innovative approaches to every aspect of synthesis and processing, characterization and measurement, and theory and computation in order 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, encompass the 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. All of the proposed IRG research is predicated on a combination of near-term and long-term scientific, technological, and societal impact. While the focus is on fundamental understanding, the knowledge that is generated, and the tools that are developed are expected to be applicable across a wide variety of problems and challenges, and are expected to have an impact that can greatly outlast the duration of the grant. Some illustrative examples in the current proposal include the TriBeam 3D imaging technique and the scanned probe diamond N-V center magnetic imaging techniques that are contributing to advancing the IRG research. Following a Seed competition, three Seed grants have started functioning since January 2018. The competition encouraged submissions on the themes of the Brain Initiative and Materials for Quantum Information. The three selected are on the topics of (i) Search for Majorana Fermions in Topological Superconductors, (ii) Perturbing Topological Crystalline Insulators with Strain, Dopants, and Ferroelectricity, and (iii) Point Defects in Boron Nitride for Quantum Information Science.

Educat**ion and Outreach:** UCSB 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. Our education programs provide undergraduate research opportunities, graduate student and postdoctoral mentoring, transferrable 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 UCSB MRSEC has the highest priority. We pay specific attention to increasing URM students at the graduate and postdoctoral levels. We have also re-competed both of our PREM relationships, with UT El Paso and Jackson State and eagerly await the results.

**Shared Experimental Facilities:** The UCSB MRSEC runs world-class shared experimental facilities which sustain and strengthen the impact of the MRSEC and related materials research within UCSB, 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 the UCSB and surrounding academic/industrial communities. In addition, we continue UCSB leadership in the growth of the Materials Research Facilities Network (MRFN), as evidenced by a recently organized MRSEC-wide SEF Workshop, further details of which will be reported in the 2019 report.

**Interaction with Industry:** The UCSB 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 **UCSB-Mitsubishi Chemical Center for Advanced Materials** (now over 15 years old, led by **Fredrickson** who also coordinates all UCSB MRSEC Industrial Outreach) and the more recently formed **Dow Materials Institute at UCSB** (led by **Hawker)** work with the UCSB MRSEC in a number of synergistic ways, and are co-located with the UCSB 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. Annually, our industrial partners meet with UCSB MRSEC faculty, graduate students, and postdoctoral researchers at a two-day symposium, the **Materials Research Outreach Program** (MROP), which was held in early February 2018; this event also involves our PREM partners, and talks appropriate for a general audience are specially advertised, illustrating the integration of all stakeholders at all levels.

**Center Management:** The management structure consists of PI and Director **Seshadri** and Co-PI and Associate Director **Jayich**), who report to the Dean of Engineering at UCSB. The Dean in turn works in close consultation with the Dean of Science, and the Vice Chancellor for Research to ensure the success of the MRSEC. **Hawker** serves as the coordinator of the SEFs, and **Fredrickson**, **Pak**, **Read de Alaniz**, and **Shea** are the other senior investigators who comprise the overall leadership team, with various responsibilities. The Executive Committee is an internal body comprising IRG Co-Leaders and all of the above individuals. The External Advisory Board comprises seven new 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 Luis Echegoyen, the founding director of the PREM at UT El Paso is retained from the previous board. All other members started in late 2015, and have played a key role in IRG selection, and more recently for selecting the successful Seeds.

**1B. Center Accomplishments for Current Reporting Period**

**Intellectual Merit**

The three IRGs of the UCSB MRSEC are off to a great start. The research being carried out in each IRG is summarized below. The IRGs are already at full staffing in terms of postdoctoral fellows, graduate students and undergraduate interns, and the first publications that acknowledge this grant have started appearing in the literature.

**IRG-1: Magnetic Intermetallic Mesostructures** focuses on structure-property relationships in intermetallics and the interrelationships between magnetism, strain, temperature, and chemistry. During the first year of this project, advances were made in establishing the necessary theoretical models for predicting magnetic ground states in composite intermetallics as well as for modeling local magnetic responses under elastic strain fields. In parallel to this, experimental advances were made in engineering strain gradients in both single phase and composite compounds as well as in mapping a bulk-averaged, renormalized magnetic response. Major advances during this reporting period include creating the first predictive framework for modeling magnetic hardening and ground state selection in solid solution Heuslers as well as the development of a high throughput screening technique for unveiling skyrmionic phase transitions in helimagnets. In particular, the IRG's work in developing techniques for engineering and modeling strain fields in both bulk and composite Heusler/half-Heusler intermetallics has set the stage for current efforts in realizing modified magnetoelastic and magnetocaloric responses in these materials.

**IRG-2: Polymeric Ionic Liquids** addresses the challenge of elucidating fundamental design principles connecting molecular architecture and charge physics with material properties in polymeric ionic liquids, with the potential to revolutionize diverse applications. IRG-2 aims to understand how materials that incorporate delocalized ionic groups onto or within a low dielectric backbone self-assemble, and how charge moves through these structures. The use of ion-exchange chemistry to impart functional properties such as photochromism, multi-valent ion conductivity, redox activity, magnetism, and reconfigurability is a key goal.

**IRG-3: Resilient Multiphase Soft Materials** is a multidisciplinary effort initiated to develop new syntheses, processing schemes, and structure-property relationships for multi-phase soft materials with resilient mechanical properties. The approach is to learn from analogous materials produced in the mussel byssus, squid beak and bloodworm jaw, a group that comprises some of the toughest and hardest known organic and composite natural materials. In particular, the team seeks to characterize 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, understand how such structuring achieves superior mechanical performance, and translate these aspects to the development of new synthetic materials and processing methods.

**Seeds:** The UCSB MRSEC is pleased to have completed its first Seed competition, with the first three successful awardees having started their Seed Projects at the beginning of calendar 2018. A flier was created that was widely distributed across the UCSB campus with the help of the Sponsored Projects Office. The flier called for proposals with wording suggesting as positive (but not exclusive) review criteria: (i) Does the proposal involve jointly-advised students and postdoctoral fellows, (ii) Does the proposal emphasize materials research relating to Quantum Information Science or the BRAIN Initiative, (iii) Is the proposed research area appropriate for NSF DMR support? (iv) Are the investigators new to the MRSEC, and (v) Will

the research advance the UCSB MRSEC vision of collaborative materials research with potential for transformative outcomes?

In addition to the reported publications, some measure of UCSB MRSEC success is seen in the recognition that UCSB MRSEC members have received during this reporting period. As a small sampling, **Fredrickson** won the Materials Theory Award of the Materials Research Society, **Pollock** was recognized by TMS through the 2018 Morris Cohen Award, and the the 2018 Alexander Scott Distinguished Service Award. **Seshadri** was the 2018 Silver Jubilee Awardee of the Materials Research Society of India. Our students have also done very well; for example Rebecca Dally (**Wilson** group) won a GMAG Dissertation Award at the APS March Meeting in 2018 for her thesis research.

**Broader Impacts**

In addition to the broader impacts of the IRG and Seed research, seen for example, in the submission of patents and the creation of start-up companies (no new start-ups during this reporting period), the UCSB MRSEC prides itself on other aspects of the way in which it interacts with stakeholders, ranging from K–12 students and teachers, through undergraduate interns, and industry partners, including local start-up companies for whom the use of the shared experimental facilities are essential for their day-to-day operations.

In terms of the education/outreach activities of the MRSEC, within this past reporting period, six programs have supported research internships at the MRSEC, including Research Interns in Science and Engineering (RISE, supported by the MRSEC), Future Leaders in Advanced Materials (FLAM, an NSF REU site), the 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). Some highlights include, in this cycle, the support of **25** UCSB undergraduate research interns through the school-year program, with **14** interns and former interns included as authors on archival publications. **7** alumni from our various programs received the prestigious NSF Graduate Research Fellowship in 2018. **9** interns presented first author presentations at conferences during the review period. In a similar vein, the new RET programs have started and are expected to impact a large number of local STEM teachers. Many other impactful activities are detailed later in this report.

The Shared Facilities of the UCSB MRSEC continue to display their usual disproportionate impact. As many as 26 publications during this (brief) reporting period acknowledge the facilities, and already, the facilities have hosted more than 93 users external to the UCSB campus, who have recharged 3800+ hours of facility use.

## 2. LIST OF CENTER PARTICIPANTS

**i. Receiving Center support:**

| | | | |
|---|---|---|---|
| Christopher Bates | Assistant Professor | Materials, Chemical Engineering | IRG-2 |
| Matthew Begley | Professor | Mechanical Engineering | IRG-3 |
| Irene Beyerlein | Professor | Mechanical Engineering, Materials | IRG-1 |
| Michael Chabinyc | Professor | Materials | IRG-2 |
| Bradley Chmelka | Professor | Chemical Engineering | IRG-3 |
| Samantha Daly | Assoc. Professor | Mechanical Engineering | IRG-1 |
| **Glenn Fredrickson** | Professor | Chemical Engineering | IRG-2 Co-Leader, IRG-3, Industry |
| **Daniel Gianola** | Assoc. Professor | Materials | IRG-1 Co-Leader |
| Songi Han | Professor | Chemistry & Biochemistry, Chemical Engineering | IRG-2 |
| John Harter | Asst. Professor | Materials | Seed |
| Craig Hawker | Professor | Materials | Facilities, IRG-2, IRG-3 |
| **Matthew Helgeson** | Asst. Professor | Chemical Engineering | IRG-3 Co-Leader |
| Ania Jayich | Assoc. Professor | Physics | Co-PI and Assoc. Director, IRG-1 |
| Robert McMeeking | Professor | Mechanical Engineering, Materials | IRG-3 |
| Kunal Mukherjee | Assistant Professor | Materials | Seed |
| Dorothy Pak | Acad. Coordinator III | Materials Research Laboratory, MSI | Education Director |
| Tresa Pollock | Professor | Materials | IRG-1 |
| Javier Read de Alaniz | Assoc. Professor | Chemistry & Biochemistry | IRG-2, Diversity Coordinator |
| **Rachel Segalman** | Professor | Chemical Engineering, Materials | IRG-2 Co-Leader |
| Ram Seshadri | Professor | Materials, Chemistry & Biochemistry | PI and Director, IRG-1 |
| Joan-Emma Shea | Professor | Chemistry & Biochemistry, Physics | IRG-3, International Programs |
| Todd Squires | Professor | Chemical Engineering | IRG-2 |
| **Megan Valentine** | Assoc. Professor | Mechanical Engineering | IRG-3 Co-Leader |
| Anton Van der Ven | Professor | Materials | IRG-1 |
| Chris Van de Walle | Professor | Materials | Seed |
| Herbert Waite | Professor | MCDB, Chemistry & Biochemistry | IRG-3 |

| | | | |
|---|---|---|---|
| **Stephen Wilson** | Asst. Professor | Materials | IRG-1 |
| Cenke Xu | Asst. Professor | Physics | Seed |

**Bold – IRG Leader/Co-Leader**

**ii. Affiliated, not receiving Center support**

| | | |
|---|---|---|
| Leon Balents | Professor | UCSB |
| Francois Barthelat | Professor | McGill University |
| Marc de Graef | Professor | CMU |
| Phillip Pincus | Professor | Physics |
| Omar Saleh | Professor | Materials, BMSE |
| Olivier Thomas | Professor | Aix-Marseille |

Abbreviations:
MSI = Marine Science Institute
BMSE = Biomolecular Science and Engineering
MCDB = Molecular, Cellular, and Developmental Biology

**iii. UCSB Faculty Members who are users of shared Center facilities (not including faculty participants receiving Center support):**

1. Mahdi Abu-Omar / Chemistry & Biochemistry
2. Stanley Awramik / Earth Sciences
3. Guillermo Bazan / Chemistry & Biochemistry
4. John Bowers / Electrical and Computer Engineering
5. Cherie Briggs / Ecology, Evolution, and Marine Biology
6. Alison Butler / Chemistry & Biochemistry
7. Irene Chen / Chemistry & Biochemistry
8. Phil Christopher / Chemical Engineering
9. Frederick Dalhquist / Chemistry & Biochemistry
10. Steven Denbaars / Materials
11. Michael Doherty / Chemical Engineering
12. Peter Ford / Chemistry & Biochemistry
13. Michael Gordon / Chemical Engineering
14. Beth Gwinn / Physics
15. Trevor Hayton / Chemistry & Biochemistry
16. Patricia Holden / Environmental Science & Management
17. Jacob Israelachvili / Chemical Engineering
18. Arturo Keller / Environmental Science & Management
19. Jonathan Klamkin / Electrical and Computer Engineering
20. Carlos Levi / Materials
21. Ben Mazin / Physics
22. Eric McFarland / Chemical Engineering
23. Gabriel Menard / Chemistry & Biochemistry
24. Umesh Mishra / Electrical and Computer Engineering
25. Samir Mitragotri / Chemical Engineering
26. Daniel Morse / Molecular, Cellular & Developmental Biology
27. Shuji Nakamura / Materials

28. Christopher Palmstrøm / Materials Science
29. Kevin Plaxco/ Chemistry & Biochemistry
30. Javier Read de Alaniz / Chemistry & Biochemistry
31. Cyrus Safinya / Materials
32. Jon Schuller / Electrical & Computer Engineering
33. Susannah Scott / Chemical Engineering
34. Mark Sherwin / Physics
35. Jim Speck / Materials Science
36. Susanne Stemmer / Materials
37. Galen Stucky / Chemistry & Biochemistry
38. Karen Szumlinski / Psychological and Brain Sciences
39. Herbert Waite / Molecular, Cellular and Developmental Biology
40. Fred Wudl / Materials
41. Andrea Young / Physics
42. Armen Zakarian / Chemistry & Biochemistry
43. Liming Zhang / Chemistry & Biochemistry

### 3. LIST OF CENTER COLLABORATORS

| Collaborator | Institution | e-mail | Field of experti | IRG Association | User of Shared Facilities |
|---|---|---|---|---|---|
| Albert, Barbara | TU Darmstadt | albert@ac.chemie.tu-darmstadt.de | Materials Chemistry | | Yes |
| Artz, Eduard | Leibniz Institute for New Materials | Eduard.Arzt@leibniz-inm.de | Materials | | No |
| Baerlocher, Christian | ETH-Zurich | baerlocher@mat.ethz.ch | Materials Science | IRG-3 | Yes |
| Betegon, Covadonga | University of Oviedo | cova@uniovi.es | Solid Mechanics | | No |
| Brown, Craig | NCNR, NIST | craig.brown@nist.gov | Neutron Scattering | IRG-1 | No |
| Davis, Thomas | Monash University | thomas.p.davis@monash.edu | Polymers | IRG-3 | No |
| De Graef, Marc | Carnegie Mellon University | mdg@andrew.cmu.edu | Electron Microscopy | IRG-1 | No |
| Díaz Rodríguez, Tania | Benemérita Universidad Autónoma, Puebla, Mexico | tgdiazr@gmail.com | Chemistry | IRG-3 | No |
| Eisenbach, Claus | Stuttgart University | eisenbach@mrl.ucsb.edu | Chemistry | IRG-3 | No |
| Fleck, Norman | University of Cambridge | naf1@cam.ac.uk | Solid Mechanics | IRG-3 | No |
| Gutekunst, Will | Georgia Tech | willgute@gatech.edu | Polymers | IRG-3 | Yes |
| Harrington, Matthew | McGill University | matt.harrington@mcgill.ca | Chemistry | IRG-3 | Yes |
| Hwang, Dong Soo | POSTECH University | dshwang@postech.ac.kr | Molecular Biology | IRG-3 | Yes |

| | | | | | |
|---|---|---|---|---|---|
| Kanatzidis, Mercouri | Northwestern University | m-kanatzidis@northwestern.edu | Materials Chemistry | | Yes |
| Kang, Wang | UCLA | wang@ee.ucla.edu | Electrical Engineering | IRG-1 | Yes |
| Kawai, Tsuyoshi | Nara Institute of Technology | tkawai@ms.naist.jp | Polymers | IRG-2 | No |
| Larsson, Josefin | KTH Royal Institute of Technology | josla@kth.se | Polymers | IRG-3 | No |
| Lawrence, Jimmy | Louisiana State University | jimmylawrence@gmail.com | Polymers | IRG-3 | Yes |
| Lee, In-Hwan | Ajou University | ilee@ajou.ac.kr | Polymers | IRG-3 | Yes |
| Lee, SangHo | Korea Research Institute of Chemical Technology | slee@krict.re.kr | Polymers | IRG-3 | Yes |
| Leighton, Chris | University of Minnesota | leighton@umn.edu | Materials Physics | IRG-1 | Yes |
| Li, Youli | UCSB | youli@mrl.ucsb.edu | Materials Research Laboratory | IRG-3 | Yes |
| Liu, Jianfang | Lawrence Berkeley National Laboratory | jianfangliu@lbl.gov | Polymers | IRG-3 | No |
| Lunn, David | Oxford University | davidjlunn@mrl.ucsb.edu | Polymers | IRG-3 | Yes |
| McCusker, Lynne | ETH-Zurich | mccusker@mat.ethz.ch | Materials Science | IRG-3 | Yes |
| McGrath, Alaina | APEEL | mcgrath.alaina@gmail.com | Polymers | IRG-3 | Yes |
| Nakano, Motohiro | Nara Institute of Technology | nakano.motohiro.na8@ms.naist.jp | Polymers | IRG-2 | Yes |
| Ni, Ni | UCLA | nini@physics.ucla.edu | Physics | IRG-1 | No |

| | | | | | |
|---|---|---|---|---|---|
| Qiao, Greg | University of Melbourne | gregghq@unimelb.edu.au | Polymers | IRG-3 | No |
| Ren, Gang | Lawrence Berkeley National Laboratory | gren@lbl.gov | Polymers | IRG-3 | No |
| Ren, Jing | Dow Electronics | jmrren@outlook.com | Polymers | IRG-3 | Yes |
| Saleh, Omar | UCSB | saleh@ucsb.edu | Materials | | No |
| Spokoyny, Alexander | UCLA | spokoyny@chem.ucla.edu | Chemistry | IRG-3 | Yes |
| Talmon, Yeshayahu | Technion | ishi@tx.technion.ac.il | Chemical Engineering | | No |
| Thomas, Oliver | Aix-Marseille University | olivier.thomas@im2np.fr | X-ray Scattering | IRG-1 | No |
| Truong, Nghia | Monash University | Nghia.Truong@monash.edu | Polymers | IRG-3 | Yes |
| Underhill, Patrick | RPI | underhill@rpi.edu | Theory | IRG-2 | No |
| Van Son, Martin | Eindhoven University of Technology | m.h.c.v.son@student.tue.nl | Polymers | IRG-3 | No |
| Walker, Lynn | CMU | lwalker@andrew.cmu.edu | Polymer Rheology | IRG-2 | No |
| Willenbacher, Johannes | BASF | jwillenbacher@mrl.ucsb.edu | Polymers | IRG-3 | Yes |
| Zones, Stacey | Chevron | SIZO@chevron.com | Chemistry | IRG-3 | Yes |

## 4. STRATEGIC PLAN

The Strategic Plan for the UCSB MRSEC in the coming year involves careful planning with regard to how the three principle "legs" of the MRSEC can involve and impact the different stakeholders, ranging from K–12 students and teachers, through undergraduate, graduate, and postdoctoral researchers, facilities scientists and faculty. The table below describes goals and desired outcomes and the quantifiable actions attempted (which also serve as metrics) for the various components of the UCSB MRSEC.

| | |
|---|---|
| **Research (IRGs)** | |
| Goal: Fostering a collaborative, interdisciplinary research culture, and creating lasting value | Strategies: Increase 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)** | |
| Pursuing new directions | Involve new investigators in the MRSEC, evolving current IRG research in new directions, and/or seed the creation of new IRGs. |
| **Facilities (SEF)** | |
| Enabling world-class research and development for UCSB, and for local industry, support efforts nationwide | Increase the number of SEF users through better publicity, increase the proportion of off-campus users, add new capabilities, and maintain fiscal sustainability, providing professional development opportunities for SEF technical staff, providing continued leadership, and help to expand the Materials Research Facilities Network. |
| **Undergraduate Education** | |
| Developing a highly trained and diverse future STEM workforce | Initiate new 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** | |
| Training for a collaborative and inclusive culture of creative research | 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** | |
| Supporting K–12 educators to incorporate materials research into curricula | Help teachers to create new curricular content that incorporates recent advances in materials and supports the Next Generation Science Standards. |
| **General public** | |
| Engaging the public with exciting new advances in materials research | Collaborate with the Wolf Museum of Exploration and Innovation (MOXI), and 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

| | | |
|---|---|---|
| Daniel Gianola | Materials | IRG Co-Leader |
| Stephen Wilson | Materials | IRG Co-Leader |
| Irene Beyerlein | Materials/Mech. Eng. | |
| Samantha Daly | Mech. Eng. | |
| Ania Jayich | Physics | |
| Tresa Pollock | Materials | |
| Ram Seshadri | Materials/Chem. & Biochem | |
| Anton Van der Ven | Materials | |

**IRG Affiliates:** Olivier Thomas (Aix-Marseille), Marc de Graef (CMU), Leon Balents (UCSB)
**IRG Postdocs:** Joya Cooley, Daniil Kitchaev, Shuozhi Xu (Elings Fellowship)
**IRG Graduate Students:** Joshua Bocarsly (NSF-GRF), Mitchell Bordelon (NSF-GRF), Alec Jenkins, Emily Levin, Simon Meynell, Flynn Walsh, Eric Yao (NDSEG), Julia Zuo (partial)
**IRG Undergraduate Students:** Julia Combs

**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:**

**Heusler/half-Heusler magnetic intermetallics.** Over the past year, IRG-1 researchers have been studying competing magnetic interactions and magnetocaloric responses in Heusler systems. Specifically, researchers have been studying a range of Heusler and half-Heusler intermetallics: as pure compounds, solid-solutions, and as designer multiphasic systems in order to understand the nature of magnetic interactions and magnetostructural coupling. This is exemplified in the investigation of the coexistence of ferro- (FM) and antiferromagnetism (AFM) in the chemically homogeneous Heusler solid solution $Mn_{1-x}Fe_xRu_2Sn$.[1] A first-principles investigation into electronic structure of the solid solution (Figure 1) suggests that FM or AFM domains form due to a competition between Sn-mediated superexchange, which favor AFM, and RKKY exchange mediated by spin-polarized conduction electrons, which favor FM.[2] Specifically, we systematically enumerated a large number of Mn-Fe arrangements over the transition metal sublattice of $Mn_{1-x}Fe_xRu_2Sn$ coupled with a similarly large number of magnetic arrangements.

The extensive first-principles calculations of the energies of different Mn and Fe orderings within $Mn_{1-x}Fe_xRu_2Sn$ coupled with different magnetic orderings were used to train an effective Hamiltonian describing chemical and magnetic disorder (i.e. a coupled cluster expansion/Ising model). The effective Hamiltonian was subsequently subjected to Monte Carlo simulations to explore the role of chemical disorder and temperature on the magnetic properties of $Mn_{1-x}Fe_xRu_2Sn$. Both Ising and Heisenberg type excitations were considered within Monte Carlo simulations and both phase diagrams show a chemical miscibility gap between $MnRu_2Sn$ and $FeRu_2Sn$ at low temperature along with continuous magnetic transitions at higher temperatures. The Mn rich Heusler exhibits antiferromagnetic ordering at low temperature while the Fe rich Heusler favors ferromagnetic ordering. The continuous degrees of freedom available to magnetic moments within the Heisenberg model lead to a dramatic reduction in transition temperatures compared to the Ising model, and taken as a whole, our experiments and models demonstrate that changes in valency upon replacement of Mn with Fe shifts the balance from superexchange-dominated interactions to RKKY-dominated interactions. This magnetic hardening in a chemically homogeneous compound has not previously been explored through first-principles computations.

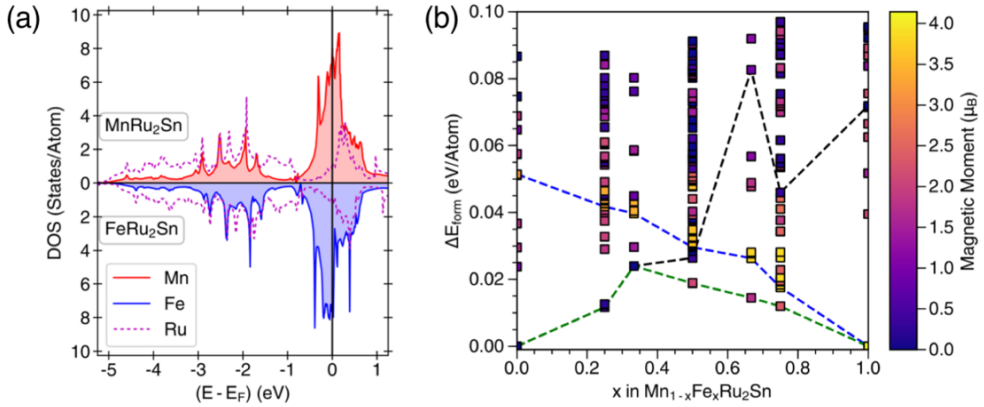


**Fig. 1**: (a) Non-spin-polarized site-projected density of states for $MnRu_2Sn$ and $FeRu_2Sn$, showing a substantial change in electronic structure near the Fermi level. (b) Formation energies of enumerated magnetic and chemical orderings of $Mn_{1-x}Fe_xRu_2Sn$ supercells. The dashed green line traces the overall lowest energy structures, showing an increase in magnetic moment with *x*.

Separately, IRG researchers have studied compositional tuning of the magnetic interactions in the $MnNi_{1+x}Sb$ Heusler system.[3] Compositions between the half-Heusler MnNiSb and full Heusler $MnNi_2Sb$ are prepared using innovative microwave synthesis, and form a solid solution with excess Ni atoms sitting on the vacant tetrahedral site in the half-Heusler structure. Atomic structure is extensively characterized using Rietveld refinement of synchrotron X-ray diffraction, and supported by DFT calculations. Magnetic interactions in the half Heusler, which are more localized than in the full Heusler, lead to stronger magnetostructural coupling as nickel content decreases, and therefore a larger magnetocaloric effect. This is accompanied by a large increase in Curie temperature, making this material highly tunable and useful in applications from magnetic refrigeration to thermomagnetic power generation from waste heat.

**Magnetocaloric response of skyrmion hosts:** IRG-1 researchers have initiated activities on characterizing/screening skyrmion hosts using the magnetocaloric effect. Skyrmion host materials show complex and subtle magnetic phase diagrams near their ordering temperatures as various topologically trivial and non-trivial phases compete energetically. In order to better understand, and ultimately control, these phase diagrams, we have developed a technique to rapidly map out the magnetocaloric effect as a function of field and temperature in high resolution. This allows for the expedient determination of phase diagrams on the basis of magnetic entropy, even at higher temperatures where heat capacity data is

dominated by lattice background. Using this technique, we are able to map the magnetoentropy of the near room temperature skyrmion host FeGe, showing that the complex magnetic signals can be understood as arising from a phase diagram containing a signal skyrmionic pocket which intersects with a line of fluctuation-driven first-order phase transitions (Figure 2). Moving forward, we plan to use this technique to study the phase diagrams of other known and new skyrmion hosts, including the polar Neél-type skyrmion host $GaV_4S_8$. In particular, we plan to use this technique to understand the effect of strain on skyrmion lattices, leveraging our IRG's unique capabilities in strain engineering.

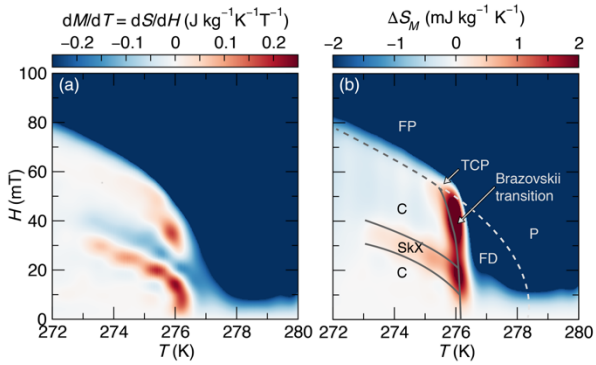


**Fig. 2**: Magnetoentropic mapping of the phase diagram of the high-temperature skyrmion host material FeGe. The DC M(T) data in (a) is transformed into the heat map in (b) using the Maxwell relation $\left(\frac{dM}{dT}\right)_H = \left(\frac{dS}{dH}\right)_T$. The isothermal magnetic entropy change, $\Delta S_M(T,H)$ is the field-integral of $\left(\frac{dS}{dH}\right)_T$. Ridges (red) and valleys (blue) in (b) indicate latent heats of field-driven phase transitions, forming the phase diagram lines shown in (c). P: paramagnetic; FD: fluctuation disordered; FP: field polarized; C: conical; SkX: skyrmion lattice, TCP: tricritical point.

**Flexomagnetism in intermetallics:** IRG-1 researchers have advanced efforts on elucidating the origins and potency of flexomagnetism – the coupling between magnetization and elastic strain gradients – on several fronts. A theoretical framework is being constructed to capture the important mesoscale features of magnetism and strain gradients. Our research has already developed powerful 3D phase field methods (PF) which are used to investigate the relation of defect elastic strain energies, applied work, and stacking fault energies, as calculated by density functional theory (DFT), to the nucleation and propagation of defects.[4, 5] The solution procedure involves minimizing a system energy functional with respect to an order parameter. The energy functional and order parameter are input into the PFDD (or any general PF) calculation and it is customary in the field of PF or solid mechanics to use equilibrium thermodynamics or Hamiltonian mechanics to define the energy functional. Gradients and any couplings between variables are determined by employing a Taylor series expansion for each term. [4,6,7]

Building from this modeling advance, researchers in IRG-1 have begun identifying experimental and computational geometries for introducing tailored strain gradients and flexomagnetic effects in single crystalline materials, enabling the measurement of both global and local magnetism owing to symmetry breaking strain gradients in their vicinity. The IRG team will carry this forward *via* crystal plasticity calculations for cylindrical holes in single crystal test specimens. The calculations deviate from the standard finite element calculation in a number of ways. The elastic strain (and stress) fields account for the crystal orientation and the anisotropy in elasticity, which can be important when the material is elastically anisotropic (Figure 3). Both displacement and orientation gradients are degrees of freedom, and these calculations will be applied to the materials of interest to tailor the needed elastic strain gradients.

Finally, the IRG-1 team has also completed the design of an apparatus for tuning strain fields and strain gradients in bulk crystals of project materials. This first-version CAD mini compression tester is capable of holding a static strain field on a test specimen for several hours, and is targeted for initial neutron diffraction studies on magnetic alloys. The device is shown in Figure 4. Immediate next steps are finalizing finite element modeling *via* ABAQUS of the system and its components and the deployment of the device in neutron diffraction studies.

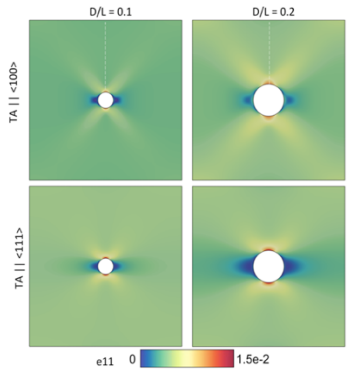


**Fig. 3**: Elastic strain fields in a single crystal containing a cylindrical hole. The strong elastic anisotropy causes the peak value and gradients to depend on the direction of tension. Note: TA = tension axis.

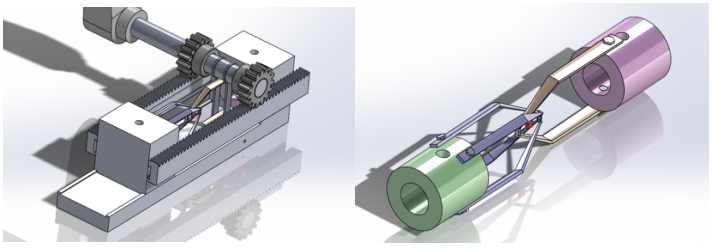

**Fig. 4**: A planned compression tester for neutron diffraction studies on Heusler alloys. Left: The entire assembly; Right: A magnified view of the inner assembly, where the sample is shown in red. The assembly is made to be highly modular.

**Research Plans:**

**Magnetostructural coupling in Laves phases:** As a near-term next step in exploring novel magnetoelastic responses in intermetallic compounds, the IRG team will begin investigating the response of Laves phase materials. These systems are typically highly frustrated magnets, and at the usually very suppressed antiferromagnetic ordering transition in geometrically frustrated antiferromagnets, the magnetic transition is frequently accompanied by a structural change that allows the magnetic ordering to take place. Unusual magnetovolume effects have been reported in $YMn_2$ where spontaneous volume magnetostriction results in a 5 % volume change at the Néel temperature. Motivated by this, IRG-1 researchers have initiated an investigation of a subset of Y-based Laves phase solid solution. The $YFe_{2-x}Co_x$ solid solution is particularly interesting, since it is a solid solution between two different magnetic ordering types ($YFe_2$ and $YCo_2$ are ferromagnetic and paramagnetic, respectively). Also of interest is substituting Cu and Zn into $YMn_2$, $YFe_2$ and $YCo_2$ ($YB_{2-x}M_x$ solid solutions in the form of solid solutions in which $B$ = Mn, Fe, and Co and $M$ = Cu and Zn). The magnetic properties of these solid solutions have not been reported. $YMn_2$, $YFe_2$ and $YCo_2$ all exist as the cubic Laves phase, while $YCu_2$ and $YZn_2$ exist as the less common orthorhombic, so studying the magnetic structure as Cu/Zn amounts are increased will be fundamentally interesting. Moreover, it has been seen that thermal expansion anomalies often occur near phase transitions. Thus, searching in this solid solution region between two different crystal structure types may prove fruitful to stabilizing phases that exhibit spontaneous volume magnetostriction.

**Advances in flexomagnetic modeling:** Very recently, we have been exploring the use of a general framework provided by non-equilibrium thermodynamics (NET) in our PFDD models, as well as our continuum models for layered structures.[8,9] This will offer another method to define the energy functional or more generally the thermodynamic potential to be used as input into PFDD. We note that NET and PFDD have important parallels. In both PFDD and NET, we seek the spatial mechanical fields as a result of non-equilibrium processes (*e.g.*, dislocation nucleation and glide, flux of dislocations, temperature effects on shear banding). Additionally, in both approaches the field variables in PFDD are functions of space and time (dislocation slip) and the basic equations are local, referring to a point in space. Therefore, for the magnetic-mechanical couplings of interest, employing NET to obtain the PFDD master energy equation will be an attractive option because the couplings between stress or strain and magnetization $M$ and their gradients ought to arise naturally without use of Taylor series expansions. In

the next year we will work toward the goal of building a new PFDD code for magneto-mechanical coupling, enabling it to use coupling coefficients from statistical mechanics and CASM calculations for the materials of interest, and applying it to specific geometries and microstructures that are experimentally tested in the laboratory.

**Magnetoelastic effects in helimagnet intermetallics.** Now that the groundwork for modeling and experimental apparatus design has been laid, a major next step for the project will be to explore the magnetic responses of candidate helimagnetic materials under applied strain. This will be accomplished at both the bulk and nanometer levels via joint strain mapping, scanning magnetometery, bulk magnetization, and neutron diffraction measurements. Materials such as MnB and FeGe, already synthesized by the project team during the current reporting period, will be explored via SQUID magnetometry and neutron diffraction under static strain fields. This will be complemented by local strain and magnetization mapping measurements via joint scanning electron microscopy and nitrogen vacancy mapping. In parallel, new materials such as the skyrmion host $GaV_4S_8$ and ferromagnetic IrMn will be synthesized for exploration via bulk strain/strain gradient studies. Scattering measurements will leverage the newly developed strain apparatus (Figure 4) and will be performed at single crystal and small angle scattering diffractometers at Oak Ridge National Lab and the NIST Center for Neutron Research. The new rapid magnetocaloric mapping technique developed for FeGe will also be employed as a high throughput screen for nontrivial magnetic states in these helimagnetic systems.

**Heusler/half-Heusler magnetic intermetallics.** In contrast to the Heusler solid solutions studied in the current reporting period, the $NbCo_{1+x}Sn$ Heusler system phase separates upon solidification, leading to a multiscale microstructure with semicoherent ferromagnetic full Heusler precipitates in a nonmagnetic half-Heusler matrix.[10] Precipitates confined within the nonmagnetic matrix show an increase in coercivity compared to pure $NbCo_2Sn$. The Heusler precipitates may exhibit this effect due to a constrained martensitic transformation, where the matrix does not allow for the magnetic easy axis to align with the applied field. The magnetic hardening, in this case, may be due to a forced magnetic anisotropy, which also likely occurs in magnetic shape memory Heuslers under confinement. This system is of potential interest for engineered control of magnetoelastic effects as well as a potential platform for exploring composite driven flexomagnetic effects. This will be actively studied in the coming year.

## IRG-2: POLYMERIC IONIC LIQUIDS

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The goal of **IRG-2: Polymeric Ionic Liquids** is to advance the fundamental understanding of self-assembly, mechanical properties, ion motion and charge physics in polymeric materials that incorporate a backbone-tethered delocalized cation (or anion) and associated counter-ion. By leveraging advanced synthetic strategies, ion-exchange chemistry, characterization tools, and theory and simulation, the design of PIL-based materials with a range of exciting functionalities can be achieved. Possible functionalities include photochromatism, multivalent ion conductivity, redox activity, magnetism and reconfigurability. The IRG-2 progress report is divided into the following themes: (i) Phase behavior of polarizable and charged polymers, (ii) Molecular design and ion transport through PILs, (iii) Strategies for modular PIL synthesis, (iv) Photoswitches for adaptable and reconfigurable PILs, and (v) Electronically conductive PILs.

**(i) Phase behavior of polarizable and charged polymers.** The chain architecture and dielectric properties of polymerized ionic liquids (PILs) are known to play an important role in determining the structure and mechanical properties, but this relationship is not well understood. The IRG team has applied a statistical field theory model for polarizable and charged polymeric systems in order to address fundamental questions about the dependence on dielectric and charge screening of the effective interactions that drive phase separation and ion aggregate formation.

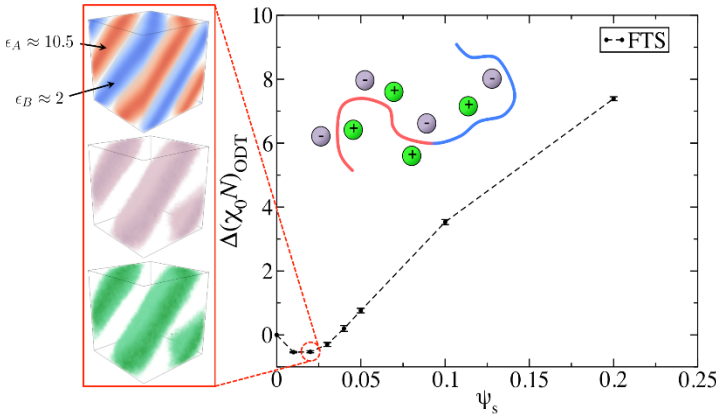



**Fig. 5.** The shift in the order-disorder transition, obtained from FTS, in a salt-doped polarizable diblock copolymer, as a function of the volume fraction of added salt.

Using analytical one-loop approximations and exact field-theoretic simulations (FTS), the dependence of the effective Flory-Huggins interaction parameter on the electrostatic environment, for a system with polarizability contrast, was elucidated. In particular, the closed-form expression for the interaction parameter, provided by the one-loop theory, describes its sensitivity to electrostatic screening. The polarizable field theory can be naturally extended to address the incorporation of charged species. An initial study on the effects of salt-doping on a polarizable diblock copolymer revealed rich behavior in which solvation, dilution and charge screening effects compete to determine whether the ordered or disordered phase is stabilized (see Figure 5). At low salt concentrations, the salt's preference for regions with high dielectric constant stabilizes the ordered lamellar phase, whereas at higher salt concentrations the combined effects of dilution and electrostatic screening by the salt stabilize the disordered phase. In the coming year, the IRG-2 team will extend this line of research to models of PILs in which the polymer chain incorporates bulky charged moieties with associated free counter-ions, in order to address the role of chain architecture and electrostatic screening in determining effective interactions and the structure of ion aggregates.

**(ii) Molecular design and ion transport through PILs.** The design of new PILs that efficiently transport ions of interest for applications such as energy conversion and stimuli response requires a deep understanding of how ions move through such complex systems.[1] We have focused on the role of metal-ligand interactions in a PIL's ability to decouple mechanics from ionic conductivity. A synthetic strategy developed by the IRG team enables precise and independent control over the nature and concentration of ligand and metal species via anionic polymerization and thiol-ene click chemistry. Tethered imidazole ligand moieties in the PIL facilitate dissociation of $Ni(TFSI)_2$ salt, forming a dynamic network with tunable modulus and relaxation timescales dependent on salt concentration. Low salt concentrations result in a simultaneous enhancement of ion conduction and mechanics, which has motivated work on understanding what molecular factors (*e.g.* ligand and ion identity, coordination geometry and timescale for metal-ligand exchange) are important in dictating ion transport and polymer mechanics/rheology. Initial work on changing the metal ion to a series of transition metals indicates that the zero-shear viscosity can be tuned over orders of magnitude while the ionic conductivity remains roughly constant (Figure 6). Further work is underway to examine the contribution of cation species to ionic conductivity. Our versatile synthetic strategy enables the expansion of our polymer library to include a variety of polymer backbones as well as tethered ligand moieties. Future work will focus on the influence of backbone dielectric constant, and both salt and ligand concentration and identity on ion transport mechanisms. We seek to identify the role of bulk dielectric constant versus local coordinating moieties on ion aggregation and mobility.

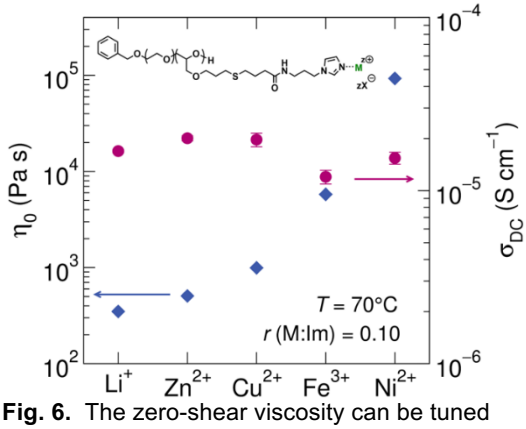



**Fig. 6.** The zero-shear viscosity can be tuned over almost three orders of magnitude with minimal changes in measured ionic conductivity.

Molecular studies are also underway to better understand the nature of interactions between metal cations to both the ligand and anion species. For the lithium-based polymer, $^{19}F$-$^{7}Li$ and $^{1}H$-$^{7}Li$ solid state NMR will be used to determine the coordination strength (via correlation spectroscopy) and relative motion (by tracking heteronuclear dipolar coupling and quadrupole coupling) of the metal ion ($Li^+$) to the PIL's imidazole site and the $TFSI^-$ anion as a function of temperature. The quadrupole pattern of $^{7}Li$ together with the heteronuclear dipolar couplings ($^{7}Li$-$^{1}H$ and $^{7}Li$-$^{19}F$) will be used to get distance and dynamics information. Electron paramagnetic resonance (EPR) spectroscopy is also being used to

determine the coordination of the transition metal counterions (*e.g.* $Cu^{2+}$, $Ni^{3+}$, $Fe^{3+}$, $Cr^{3+}$, $Gd^{3+}$) to the PIL ligand sites and $TFSI^-$. CW EPR lineshape analysis can determine metal counterion clustering (Figure 7 suggests $Cu^{2+}$ clustering), and pulsed EPR Hyscore will be used to determine distances (2 Å to 5 Å) and detailed orientation between the transition metal ion and both the $TFSI^-$ *via* $^{19}F$ ($I = 1/2$) and PIL imidazole site via $^{14}N$ ($I = 1$).

**(iii) Strategies for modular PIL synthesis.** Recognizing nature's ability to achieve materials through precise, discrete molecular design, the IRG team is developing synthetic and supramolecular strategies that access multiple polymer backbones and architectures with control over functional groups for ionic or hydrophobic interactions. Two major themes have been explored this year: development of new synthetic approaches to ionic materials and the identification of assembly processes that may be compatible with the controlled incorporation of ionic liquid (IL) building blocks.

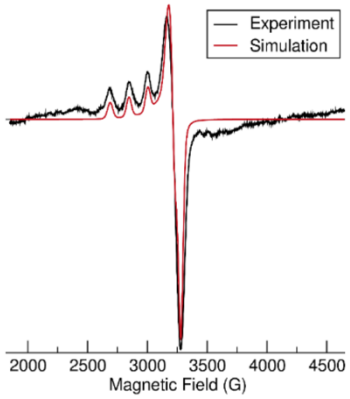



**Fig. 7.** X-band cw EPR (black) and simulated (red) spectra at 300 K of the $Cu^{2+}$/PIGE/TFSI system. The broadening observed is potentially due to clustering of $Cu^{2+}$ ions.

Combining controlled polymerization with the identification of new building blocks for PILs, we have developed a simple and efficient transformation of thiol and thiocarbonylthio functional groups to bromides using stable and commercially available brominating reagents. Bromo chain end groups are much more applicable for introduction of ionic groups through quaternization reactions with a wide variety of N-containing derivatives. This procedure allows for the quantitative conversion of a range of small molecule thiols (including primary, secondary and tertiary) to the corresponding bromides under mild conditions, as well as the facile chain-end modification of polystyrene (PS) homopolymers and block copolymers prepared by reversible addition–fragmentation chain transfer (RAFT) polymerization. Specifically, direct chain-end bromination of PS prepared by RAFT was achieved, where the introduced terminal bromide remained active for subsequent modification using classical atom transfer radical polymerization (ATRP).[2] This transformation sets the foundation for bridging RAFT and ATRP, two of the most widely used controlled radical polymerization (CRP) strategies and enables the preparation of chain-end functionalized block copolymers not directly accessible using a single CRP technique. This work highlights the significant potential for introduction of single or multiple ionic groups at specific points in common vinyl-based polymers.

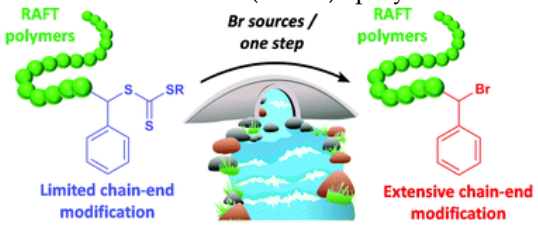
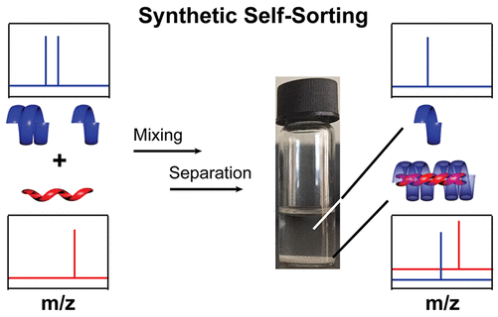



**Fig. 8.** Graphical representation of the mild, user friendly chemistry developed for transforming a RAFT chain end to a synthetically more useful bromo chain end.

The triple-helix stereocomplex of poly(methyl methacrylate) (PMMA) is a unique example of a multistranded synthetic helix with significant utility in nanotechnology and materials science. The controlled placement of IL building blocks within these assemblies (*i.e.* outer surface versus internal or end areas) would facilitate the use of IL-based materials in bio-inspired nanostructures (*i.e.* viral capsid formation). To gain a fundamental understanding of the underlying assembly process, discrete stereoregular oligo(MMA) libraries were prepared by combining stereospecific polymerization techniques with automated flash chromatography purification.[3] Stereocomplex assembly enabled the identification of the minimum degree of polymerization required for stereocomplex formation and the dependence of the helix crystallization mode on the length of assembling precursors. Significantly, our experiments resolved binding selectivity between similar molecular weight helical strands, presenting opportunities for

the design of polymeric materials in which ionic units are included in the oligio(MMA) precursors and are specifically localized in the final triple helix nanostructure.




**Scheme 1.** Illustration process for molecular weight-based self-sorting of linear polymer chains through triple helix formation.

We will use these synthetic schemes (such as the one displayed in Scheme 1) to develop new approaches to soluble polymers and crosslinked networks incorporating IL building blocks. A key area of interest is in silicone-based systems using novel boron-catalyzed addition chemistry that is orthogonal to traditional functionalization approaches. We will also continue to explore supramolecular assembly processes, such as triple helix formation, with ionic assembly.

**(iv) Photoswitches for adaptable and reconfigurable PILs.** To develop strategies to transform PILs into adaptive and reconfigurable materials, we plan to use light-responsive molecules such as photoacid, photobase, or photometal generators to affect the physical properties of the polymer in the illuminated regions. During this funding period new photoswitches were synthesized that can release $H^+$ upon exposure to light, as well as photoswitches that will alter the aromaticity and metal-ligand coordination strength of the pendant imidazole (Figure 9). These initial investigations have established a few important design principles that will guide our future strategy. For example, the incorporation of *tert*-butyl groups on the photoacid increased the solubility of the photoacid 5-fold compared to previous photoacids.[4] Solubility of previously reported photoacids [5] is a major limitation that now can be overcome with the new photoacid. Additionally, the imidazole bearing a diarylethene as a photoswitching unit can be incorporated into systems currently under investigation.

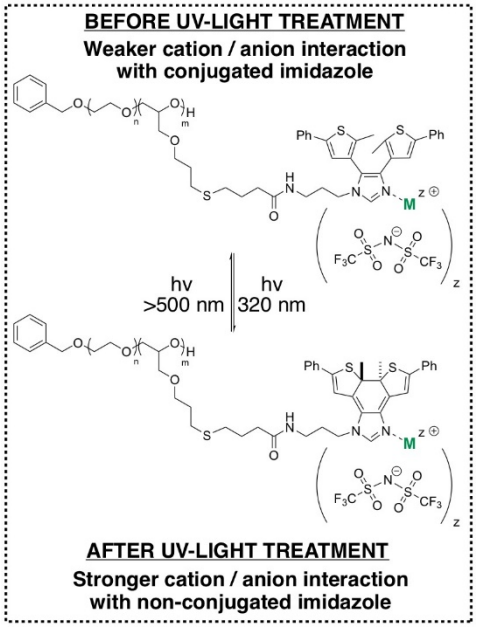



**Fig. 9.** Photoswitch-based imidazole group that can alter the metal-ligand coordination.

With these photoswitching molecules in hand, we are now positioned to begin to investigate light mediated changes in physical properties of PILs on demand and with spatial resolution. However, we will simultaneously continue the further optimization of the reversible photoacid system to identify related photometal generators, as well as photoacids with pKa's that expand our compatibility with current PILs. As described above, it has been demonstrated that the rheology and ionic conductivity of PILs are distinctly influenced by metal-ligand coordination. Building on this work, we will use PILs bearing photoswitch-based imidazole groups to manipulate the metal-ligand coordination upon light irradiation and investigate the influence on both polymer viscoelasticity and the rate at which ions can be transported.

(**v) Electronically conductive PILs.** The design of polymeric materials with low glass transition temperatures ($T_g$) that allow electrical an charge to hop along the polymer chain could lead to truly elastic conductive materials. To this end, we have begun to characterize a benchmark amorphous polymer with electrical conductivity along the main chain and to design polymers with redox-active pendant groups.

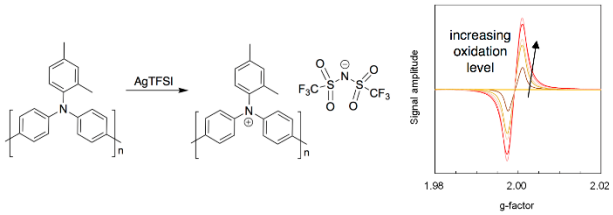



**Fig. 10.** PTAA can be oxidized with AgTFSI in solution. Solid samples show increasing spin concentration with the level of oxidation suggesting the formation of polaronic charge carriers.

In an initial project, the behavior of an amorphous poly(triarylamine) (PTAA) polymer has been examined to determine if its oxidized backbone can be solubilized with a bulky molecular anion, $TFSI^-$ (Figure 10). While the majority of conductive polymers are poorly soluble upon oxidation, PTAA remains highly soluble in common organic solvents upon oxidation with AgTFSI. Furthermore, we find that the $T_g$ of PTAA increases only slightly (from ≈ 147 °C to 149 °C) at relatively high levels of oxidation (≈1/10 monomers) with $TFSI^-$ as a counter-ion. Electron spin resonance is consistent with the formation of charge carriers with spin ½ and the resulting solid films have conductivities of ≈ 0.1 S/cm. This materials system shows the potential of diffuse/bulky counter-ions to enhance the processability of conductive polymers.

Our initial design strategy to develop new conductive PILs is to synthesize flexible chain polymers functionalized with redox active pendant units. Partial oxidation of these pendant units will allow charge hopping between sites. MMA-based polymers with phenothiazine pendant groups by co-polymerizing two monomers (Figure 11) have been synthesized. This design strategy allows us to control the density of redox-active pendants along the backbone by controlling the monomer feed ratios and to further lower the $T_g$ by modifying the co-monomer, e.g. butyl acrylate. The IRG team is currently determining efficient oxidation chemistries to introduce $TFSI^-$ counter-ions into the phenothiazine polymers. We plan to study the dynamics of charge hopping and ion motion in these materials using a combination of impedance and solid-state EPR measurements. We will determine the trade-off between functional group density, which is expected to enhance electrical conductivity, and thermal properties, such as $T_g$, towards the development of soft conductive PILs.

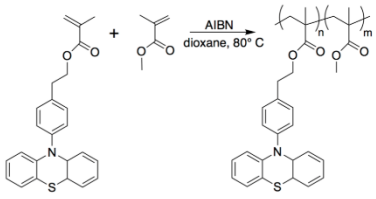



**Fig. 11.** Monomers with pendant phenothiazine groups can be co-polymerized with methyl methacrylate.

## IRG-3: RESILIENT MULTIPHASE SOFT MATERIALS

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| Glenn Fredrickson | Chem. Eng./Materials | |
| Craig Hawker | Materials/Chem. & Biochem. | |
| Robert McMeeking | Mech. Eng./Materials | |
| Joan Emma Shea | Chem. & Biochem./Physics | |
| Herbert Waite | MCDB/Chem. & Biochem./BMSE | |

**Additional faculty involvement**: Francois Barthelat (McGill University)

15 Postdoctoral Associates and 17 graduate students (heavily leveraged with external fellowships)

**Postdoctoral researchers:** Bas van Ravensteijn, Daniel DeMartini, Christophe Monnier, Keila Cunha Silva, Noy Cohen, Jing Ren, Jimmy Lawrence, Abby Knight, Raghida Bou Zerdan, Bernd Oschmann, David Lunn, Athina Anastasaki, Morgan Schulze, James McCarty, Emmanouela Filippidi

**Graduate students:** Scott Fenton, Tuan Nguyen, Rubayn Goh, Brad Killingsworth, Teodora Losic, Eric Valois, William Wonderly, Jamie Booth, Allison Abdilla, Adam Levi, Emre Discekici, Anna Melker, Jan Garcia, Nathan Prisco, Marcela Areyano, Luke Gockowski, Aimal Khankhel (NSF GRF)

**Undergraduate researchers:** Olivia Konttinen, Koe Imlow, Josphine Larsson, Shay Seguin, Remy Vrahas, Shelby Shankel, Justin Bernstein, G. Chandler Bartz

Research in IRG-3 during the current reporting period falls along three broad themes: (i) natural and synthetic chemistries for self-assembly and bonding, (ii) understanding and controlling non-equilibrium processing, and (iii) mechanics of bio-inspired adhesives.

### (i) Innovations in natural and synthetic chemistries for self-assembly and bonding

**i.a Discovering the role of melanin synthase in constructing load-bearing bloodworm jaws.** The bloodworm, *Glycera dibranchiata*, has strong, wear-resistant jaws composed of a glycine and histidine rich protein, copper (in mineralized and ionic form) and, surprisingly, *melanin*, which is contiguous throughout the jaw. Thus, it is the only known load-bearing melanin. The IRG team is leading efforts to identify and determine the role of proteins into melanin self-assembly into large, load bearing structures. Next-Generation RNA sequencing identified melanin synthase, with an active site of copper-coordinated histidine, which was subsequently cloned and expressed in *E. coli* in mg amounts, allowing unprecedented analysis of its biochemical and structural properties. Its catalysis and thermodynamics of metal binding were determined by Michaelis-Menten kinetics (Figure 12) and isothermal titration calorimetry, respectively. Surprisingly high enzymatic activity was found, and catalysis products were visualized by optical, electron and atomic force microscopy, revealing that the synthase mediates melanin assembly into robust well-defined sheets with thickness of ≈ 40 nm and modulus of ≈ 8 GPa (Figure 12). Taken together, our results show that melanin synthase possesses unprecedented ability to: catalyze Dopa oxidation, to template melanin structures, and to assemble into a separate, but melanin-associated, polymer network. These exciting discoveries lay an important foundation that we will build upon in future years. Planned

experiments include real-time analysis of protein self-assembly and determination of the 2D sheet structure, mechanics and chemistry including possible stratification, which will be complemented by molecular modeling of melanin-copper, protein-copper, and protein-melanin interactions.

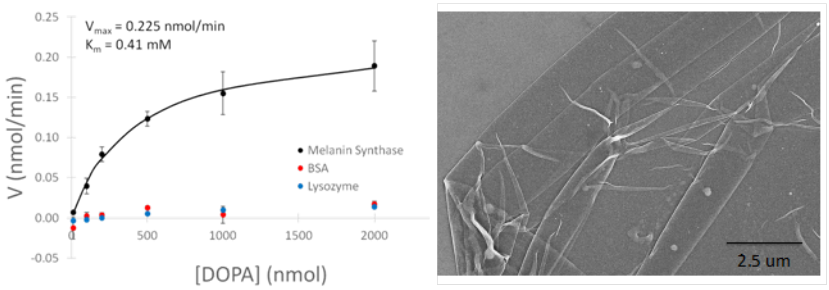


**Fig. 12.** (left) Plot of kinetics data of melanin synthase acting on DOPA. (right) Scanning electron micrograph of nanosheets formed by melanin synthase.

**i.b. Bioinspired synthetic polymers with novel sequence specificity, assembly and bonding.** Recognizing nature's ability to achieve materials through precise, discrete molecular design, a collaboration with IRG-2 members is developing synthetic strategies to access polymer architectures with control over functional groups for ionic or hydro-phobic interactions (*e.g.* for coacervation), and reactive groups for covalent and non-covalent (*i.e.* H-bonding, ionic) crosslinking. The scope and accessibility of sequence-controlled multiblock copolymers was recently demonstrated by direct *in situ* polymerization of hydrophobic, hydrophilic and fluorinated monomers. Key to the success of this strategy is the ability to synthesize ABCDE, EDCBA and EDCBABCDE sequences with high monomer conversions (>98 %) through iterative monomer additions, yielding excellent block purity and low overall molar mass dispersities (Đ<1.16). Small-angle X-ray scattering showed that certain sequences form well-ordered mesostructures.[1] This approach constitutes a simple versatile platform to expand the availability of tailored polymeric materials from readily available monomers, and affords spatiotemporal control compatible with the proposed processing/characterization methods to be developed in IRG-3.

The IRG team expanded on these recent advances to address how length and functional unit distribution (random vs. defined) influence phase behavior and self-assembly properties. Inspired by marine systems that deliver material precursors through vesicular structures that exhibit morphological shifts upon metal coordination, hybrid peptide-polymer conjugates with metal ion coordination-sensitive morphology were designed (Figure 13). Coupling of a peptide chelator, hexahistidine, with hydrophobic oligo-styrene allows a modular strategy to be established for the efficient synthesis and purification of these tunable amphiphiles (oSt(His)6). Remarkably, in the presence of different divalent transition metal ions a variety of morphologies were observed.[2] This work highlights the significant potential for transition metal ion coordination as a tool for directing the assembly of synthetic nanomaterials and will be further exploited in other IRG-3 systems in future work.

The IRG team incorporated mussel-inspired sacrificial, reversible iron-catechol cross-links into a dry, loosely cross-linked epoxy network that is remarkably stiff *and* extensible.[3] The iron-containing network imparts multiple orders of magnitude increases in stiffness, tensile strength and toughness compared to iron-free analogues as well as recoverable hysteretic energy dissipation and sustained extensibility. Compared to previous realizations of this chemistry in hydrogels, the dry nature of the network enables larger property enhancement owing to the cooperative effects of both increased cross-link density given by the reversible iron-catecholate complexes and the chain-restricting ionomeric nanodomains that they form. IRG members and collaborators also created mussel-inspired molecular primers that substantially increase the adhesion strength of crosslinked polymethacrylate resins, with applications to dental restoration and other structural materials.[4]

In the forthcoming year, these synthetic schemes will be used to develop peptides and water-soluble polymers that mimic essential biochemical motifs to perform a range of critical functions. This includes triggered coacervation and phase separation *via* environmental stimulus, such as pH (*e.g.* using the pKa of histidine), temperature (*e.g.* using hydrophobic residues) or ion addition (*e.g.* multi-valent transition metals). Physical bonding will be explored to arrest the phase separation and reinforce internal interfaces, *e.g.* through catechol and imidazole groups (by metal complexation, H-bonding, or interfacial adhesion). Dopa will be introduced using functionalization of thiol-containing synthetic peptides/polymers with eugenol derivatives *via* click chemistry. In particular, new chemistries will target the triggered formation of porous and multi-phase morphologies with mesoscale structure through arrested phase separation, in conjunction with the efforts described below on non-equilibrium processing.

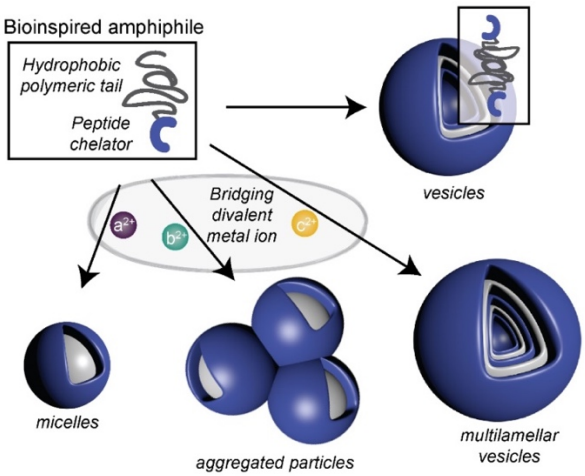


**Fig. 13.** Schematic illustrating a single amphiphillic material that can be transformed into a variety of unique morphologies in response to the presence of different divalent transition metal ions.

**i.c. Model system development to understand how molecular interactions drive coacervation**
Coacervation is a conserved process across our exemplar natural materials for the formation of multi-phase, physically bonded networks. To better understand and mimic the basis for coacervation, the polymer field theoretic simulation (FTS) approaches have been developed to study intrinsically disordered proteins (IDPs) including mussel foot proteins/peptides, which offer unique opportunities to study polymers with controlled, monodisperse and non-random heterogeneous sequences.[5] In a collaboration with IRG-2, it was demonstrated that such peptides are effective pressure-sensitive wet adhesives.[6] To better understand the relative contribution of charge sequence, polymer charge density, salt concentration, and polymer excluded volume on the phase behavior, a minimal polyelectrolyte model that includes the relevant physical requirements of chain connectivity and sequence dependent charges has been adopted. To bridge to atomistic simulations, a new set of molecular simulations with coarse-grained interaction parameters for peptides and peptoids consistent with the GROMOS force field have been developed that provide a direct input to FTS simulations. Initial combined studies focused on simplified proteins with cationic lysine and anionic glutamate residues that differ in the sequence of charges along a fixed overall charge density or net charge (Figure 14). Significantly, we find that the presence of larger like-charged 'blocks' favors coacervation, providing an important testable hypothesis and input for experimental synthetic designs. In upcoming years, the FTS model will be updated to incorporate more specific amino acid interactions, allow dipole interactions and introduce hydrophobic effects explicitly. Coarse-grained atomistic simulations will be generalized to other biomolecular force fields, and extended to allow prediction of interfacial interactions to guide experimental designs in multi-phase materials.

First steps toward testing these results involve peptoids with N-substituted glycine oligomers recently synthesized in a collaboration with IRG-2. Translation to more available synthetic polymers through synthetic schemes for controlled living radical polymerization and subsequent functionalization will produce quaternary ammonium and carboxy-substituted polyacrylates. In the coming year, these polymers will serve as model systems for testing the predictions, and will serve as a platform for building additional bonding and structuring schemes for non-equilibrium processing.

**(ii) Innovations in understanding and controlling non-equilibrium processing**

**ii.a Determining the time-dependent processing strategies used to form porous structures in mussel adhesive plaques**. The mussel byssal holdfast forms a disk-shaped plaque that is responsible for its function as an exceptional adhesive. In several species (i.e. *Mytilus californianus, Mytilus galloprovincialis*) the internal plaque architecture is a porous protein foam interpenetrated by collagen fibers. It has been hypothesized that this foam imparts toughness through collagen pullout and scission as well as pore fracture, and that the foamy architecture may additionally hinder crack growth.[7] Learning how the mussel processes this foamy structure will provide critical design considerations for non-equilibrium processing of synthetic materials. It was recently found that the solid plaques are formed within several minutes of the injection of soluble, prepackaged proteins that undergo phase separation and crosslinking. Although the protein composition in mature plaques is largely understood,[8] very little is known of how the complex structures are initially formed or the role of metal ions in structural maturation. Electron microscopy and amino acid analysis are establishing the role of seawater composition on plaque maturation. Porosity formation is found to occur within ≈ 30 min of deposition. Submersion in neutral to basic pH is required, and the presence of $Ca^{+2}$ influences the final architecture. This suggests the importance of electrostatic interactions and water in the phase transformation dynamics. In other ongoing work, a comparative approach will investigate whether different mussel species subjected to differing ocean loading conditions produce plaques and threads of differing composition, internal structure, and mechanics. Results will provide a basis for the synthetic designs for phase transformation triggers for non-equilibrium processing, informing modeling of mussel plaque mechanics.

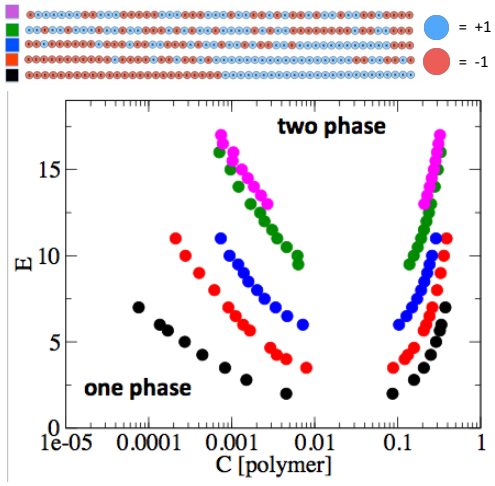


**Fig. 14.** FTS predicted phase coexistence boundaries for coacervation of sequence-defined lys-glu co-polymers in solution. E and C characterize the fluctuating electrostatic field strength and polymer density.

**ii.b. Development of new electrochemistry approaches to study mussel adhesive formation** Electrochemistry has a significant untapped potential to characterize the interfacial chemistry of mussel plaques using the redox of 3, 4-dihydroxyphenyl-L-alanine (Dopa) as a reporter. Mussels were presented with gold foil that served as both a substrate for attachment and a working electrode for interfacial analysis by cyclic voltammetry (CV). Under seawater conditions only trace amounts of Dopa were observed due to the poor solubility of adhesive mussel foot proteins. However, in 0.15 M acetic acid, the dissolution of Dopa-containing interfacial Mfps was detected with time-dependent currents peaking at an oxidation potential of +0.53 V. In combination with TEM, electrophoresis and mass spectrometry, these results indicate that mature plaques contain significant levels of interfacial mussel foot proteins (*e.g.* Mfp-6, Mfp-3) in insoluble form, but not as covalently cross-linked proteins (Figure 15). Such phase-separated compartments may reveal a key role for the network found within the small pores of the plaque - by

insulating Dopa-containing proteins against seawater mediated oxidation and polymerization. In coming years, these experiments will be expanded to track the time evolution of plaque processing by combining viscometry of the plaque fluid and fast CV scans with liquid phase electron microscopy (ending expansion of UCSB SEFs through a submitted NSF MRI award).

**(iii) Innovations in mechanics of bioinspired adhesives**

Initial experimental, analytical and computational approaches to understand multi-scale mechanics of resilient soft materials have focused on understanding how the geometries and design features found in natural load-bearing materials impact performance of bioinspired adhesive mimics. **Valentine** has pioneered the use of 3D printing and injection molding to create mussel-inspired silicone structures (Figure 16). This work opens new studies to explore the role of dissipation and non-affine deformations at interfaces in determining strength, toughness and detachment, as it is possible to directly image the millimeter scale elastic structures during loading. Future work will explore loading of asymmetric structures, as well as use of multiphase or composite materials to introduce internal modes of dissipation. A partnership with IRG-1 to develop digital image correlation approaches to better characterize the 3D deformation field has been initiated. Computational models will allow determination of structure detachment force as a function of the separation distance between the adhered surface and the rigid substrate and therefore as a function of adhesion energy and structure geometry. A significant aim of the modeling will be to understand the transition from abrupt detachment to peeling, and the manner in which geometric design may be invoked to provide the highest possible adhesion strength for a given angle of attack.

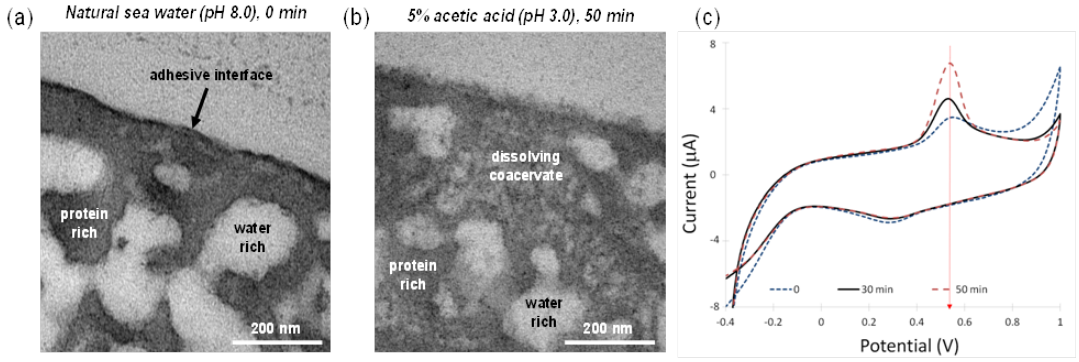


**Fig. 15**. (a) Mature mussel byssal plaque collected from seawater exhibits a foamy structure that transforms when equilibrated for 50 min in acetic acid (b). (c) CV on plaques deposited onto gold with Dopa as a reporter for Mfp-3 tracks the reversible solubilization of Mfp-3 from an insoluble phase (coacervate), indicated by the increasing current at 0.53 V.

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## SEEDS

### SEED: SEARCH FOR MAJORANA FERMIONS IN TOPOLOGICAL SUPERCONDUCTORS

John Harter Materials
Cenke Xu Physics

Majorana fermions—exotic particles that are their own antiparticles—are predicted to appear in a special class of superconductors called topological superconductors. These emergent quasiparticles have attracted excitement as possible building blocks for a fault-tolerant "topological quantum computer" that is immune to environmental decoherence. Two materials, $Nb_xBi_2Se_3$ and $FeTe_{1-x}Se_x$, have recently shown promise for hosting a topological superconducting phase. $Bi_2Se_3$ is the archetypal topological insulator, exhibiting a single Dirac surface state at the Γ point. When doped with a metal like Nb, the material becomes superconducting. Nuclear magnetic resonance and torque magnetometry experiments suggest that the superconducting state is topological, with odd-parity spin-triplet Cooper pairing. $FeTe_{1-x}Se_x$ is a new candidate topological superconductor; very recent angle-resolved photoemission spectroscopy and scanning tunneling microscopy studies measured a proximity gapping of the topological surface state and detected Majorana bound states at vortex cores, respectively. In this seed project, bulk single crystals of $Nb_xBi_2Se$ and $FeTe_{1-x}Se_x$ will be synthesized (under the supervision of collaborator Stephen Wilson) and characterized to ensure chemical homogeneity and large superconducting volume fractions. After growth, the superconducting order parameters and Majorana modes of the samples will be studied using optical second harmonic generation (SHG) and magneto-optical microscopy. SHG is an ideal tool for studying odd-parity (*e.g.* p-wave) Cooper pairing—a prerequisite for topological superconductivity—because leading-order electric dipole SHG is forbidden in a centrosymmetric material. The order parameter of a topological superconductor spontaneously breaks inversion symmetry, thereby making SHG a direct and sensitive probe of its presence. SHG will be measured in these materials to search for signatures of this symmetry breaking below the superconducting critical temperature. Additionally, a magneto-optical microscope will be constructed to both image and manipulate superconducting vortices, necessary for braiding Majorana bound states to perform topological quantum computations (see Figure 16). To complement experiment, theoretical work will be performed under the supervision of co-PI Cenke Xu to investigate the interaction effects between multiple Majorana zero modes in proximity to one another, especially in the relatively strongly correlated superconductor $FeTe_{1-x}Se_x$, as well as the potentially nontrivial interplay between strong interactions and topology.

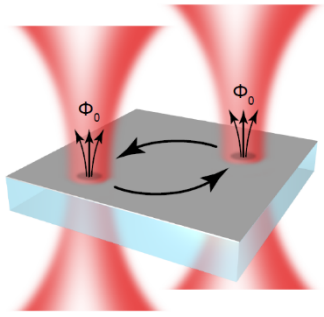



**Fig.16**. Illustration of optical manipulation of flux quanta in a topological superconductor. Vortices that bind Majorana zero modes are pinned by hot spots generated by two focused laser beams. By moving the laser spots, the vortices (and therefore the Majorana bound states) can be braided around each other.

## SEED: PERTURBING TOPOLOGICAL CRYSTALLINE INSULATORS WITH STRAIN, DOPANTS, AND FERROELECTRICITY

Kunal Mukherjee Materials

This seed proposal aims to demonstrate precise control over the properties of quantum materials by understanding the role of structure. This will be performed using thin films grown by molecular beam epitaxy (MBE). This seed project aims to elevate research in the field of quantum materials leveraging advances in semiconductor growth and junction physics. Topological crystalline insulators (TCI) are a recently discovered phase of quantum matter that has exotic Dirac surface and interface states protected by crystal symmetry. Over the next 2 years, we plan to systematically induce strain, introduce dopants, and study the onset of ferroelectric ordering towards breaking this crystal symmetry.

In the coming year, the seed will fund a graduate student to synthesize and characterize thin films of the IV-VI (Pb,Sn)(Se,Te) family of TCI materials with atomic layer-by-layer control. The MBE is slated for installation in May 2018 (See Figure 17). We have acquired 6N (99.9999%) purity chemicals and high-quality crystalline substrates. We also expect to complete preliminary characterization of films by electron microscopy and to start transport measurements at the shared facilities of the materials department and the MRSEC.

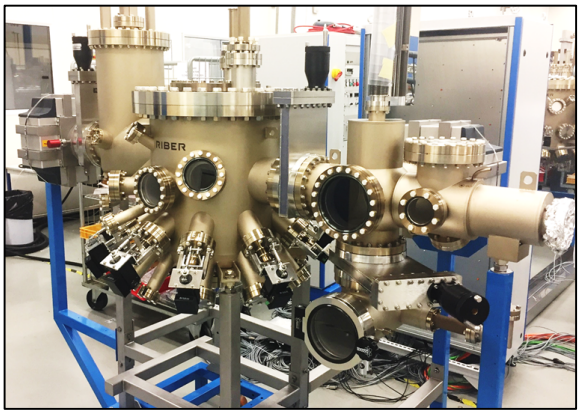



**Fig. 17.** The molecular beam epitaxy chamber for topological crystalline insulator growth awaiting installation in the PI's lab.

**SEED: POINT DEFECTS IN BORON NITRIDE FOR QUANTUM INFORMATION SCIENCE**

Chris Van de Walle Materials

Collaboration with: Ania Jayich, Physics, UCSB (unfunded) and Audrius Alkauskas, FTMC, Vilnius, Lithuania (unfunded).

Point defects in semiconductors have emerged as leading platforms for quantum information technologies including quantum memories, repeaters, simulators, and sensors. The most prominent example is the NV center in diamond (a complex between a vacancy and a substitutional nitrogen at-om), which has been widely studied as a qubit and as a single photon emitter. Although the NV center serves as the prototype, it is far from ideal, mainly because diamond is difficult to grow and process, and because the NV center efficiency is quite low. The search is underway to identify point defects in other host materials whose characteristics exceed those of the NV center. Experiments have identified promising single-photon emitters in hexagonal BN, a two-dimensional (2D) material. However, the microscopic origin of the SPEs has not yet been identified. It is also unclear whether the light-emitting centers are also spin centers, i.e., whether they can serve as qubits or as sensors of magnetic fields. In addition, there are concerns about whether coupling to phonons in extremely thin 2D materials might be an obstacle for reaching high optical efficiencies. The goal of the proposed project is to elucidate these fundamental issues through a combination of first-principles calculations and experimental characterization. Calculations have already been initiated on formation energies and charge-state transition levels of candidate defects. In parallel, an investigation is being carried out to investigate how the electronic structure of BN evolves as a function of the number of layers in a stack.

## 6. EDUCATION AND HUMAN RESOURCES

### CURRENT ACTIVITIES

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 stake holders; CAMP, CISEI, FLAM and PREM are all at least partially funded from other NSF awards. In addition, every summer several students are partially funded by MARC, individual PI award supplements, or the UCSB College of Engineering, although they participate fully in our summer program. Due to the dates of this report, we report only on the outcomes of students who participated during the fall and winter quarters of 2017 and 2018.

*Future Leaders in Advanced Materials (FLAM), Research Interns in Science and Engineering (RISE) and PREM*
The RISE program supports school year internships for UCSB students. RISE students are placed in research laboratories and assigned a personal mentor, usually a graduate student or postdoctoral researcher. Students also participate in regular intern group meetings, practice giving oral presentations on their research, and produce final written and oral reports. Students also have the option of participating in career development activities (reported below). In this cycle we supported **25** UCSB undergraduate research interns through the school-year RISE program. **14** interns and former interns were included on refereed publications in this cycle (listed below). **7** alumni from our various REU programs (including FLAM, CAMP and CISEI) received the prestigious NSF Graduate Research Fellowship in 2018. **9** interns presented first author presentations at conferences during the review period.

*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** | **# Participants** |
|---|---|---|
| Peer Study Group | Fall, Winter | 75 |
| Applying for Internships | Fall | 19 |
| Graduate Student Panel and Workshop | Summer, Fall | 67 |
| Applying for the NSF GRF | Fall | 15 |
| Oral Presentation Workshop | Winter | 25 |
| Northrop Grumman Workshop | Winter | 15 |

**UCSB MRSEC Teacher Programs**

*Research Experience for Teachers (RET).*

The RET program is modeled on undergraduate research programs and serves local secondary science teachers. Summer 2017 marked the program's nineteenth 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.

Unlike the undergraduate programs, the RET program is a two-year commitment. 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 might 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 where they present their projects to secondary teachers from the two-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. Four RET I teachers were funded by the UCSB MRSEC to pursue research projects. Four teachers developed lesson plans under RET II and will present them at the March 16, 2018 UCSB MRSEC Secondary Curriculum Workshop. Over 70 local science teachers are registered to attend. All RET lesson plans and curriculum materials are available online on the UCSB MRSEC website (http://www.mrl.ucsb.edu/RET). As of February 2018, 71 curriculum projects are archived. A 2008 survey of RET alumni indicates that 80% of the projects are still in use, indicating a lasting impact on teaching methods.

**Informal K-12 Education**

*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. An outgrowth of ScienceLine includes video interviews, answers and presentations, and YouTube-style videos on topics in Materials Science (http://www.mrl.ucsb.edu/education/resources-teachers). In 2017 we received 509 questions bringing the total archived questions and answers to 5967. ScienceLine is designed to primarily serve local schools and teachers; in 2017 students from over 150 different California schools submitted questions. Overall, questions were received from over 350 different schools, both US and international (not all users specify their school). In 2017, 63 UCSB scientists, including faculty, postdocs, graduate students, undergraduates and alumni participated by answering questions. Fifteen of the participating scientists were from the UCSB MRSEC.

*Family Science Nights/It's a Material World*

In spring 2006 the UCSB MRSEC introduced a set of hands-on exhibits of new materials designed for presentation to K-6 students and their families in an informal setting. During the 6-month review period, we presented It's a Material World at Family Science Nights at six local elementary to over 900 students and their families. It's a Material World was presented by 31 UCSB MRSEC graduate student and postdoc volunteers.

*Build your own Buckyball*
In 2007 Ram Seshadri and Education Director Dorothy Pak received a Faculty Outreach Grant 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. During the 6 month review period we presented the activity to 70 elementary school students, assisted by 3 graduate student volunteers.

*Solar Car Workshops*
In 2011 UCSB MRSEC Director Ram Seshadri and Education Director Dorothy Pak received a FOG grant to develop a new hands-on workshop on alternative energy and photovoltaics. During the 6 month review period, 65 elementary, middle and high school students and their families participated in the workshop, assisted by 10 graduate student, post doc and faculty volunteers. In particular, we partner with the UCSB Office of Education Partnerships to present the workshop to students from UCSB partner schools with high minority enrollments and low college-going rates, including the MESA Science and Technology Day, which brings over 1000 underrepresented minority middle school students to campus in March.

*Maker Activities*
In order to meet our local teachers' needs for "Maker" activities we have developed hands-on, inquiry-based activities focused on Bio-inspired soft robotics. During the 6-month review period, we presented these activities at 3 schools to over 300 elementary and middle school students with 27 undergraduate, graduate and postdoctoral volunteers. We have two additional school Maker Faires planned in the next two months.

*Other K-12 Activities:*
We make a priority of meeting teachers' needs and requests for science fair judges, classroom presenters, science expert panelists and presenters at career fairs. Over the review period we provided volunteers and activities at five such events, interacting with approximately 200 K-12 students.

**Education Program REU and RET Projects September 2017-February 2018**

***RISE School Year Participants***
**Abel Flores-Prieto**, UCSB, Mentor and PI: Omer Blaes, "Modeling the frequency spectrum of AM CVn systems by solving the radiative transfer equation"

**Abhilasha Kumar**, UCSB, Mentor: Adam Lucio; PI: Otger Campas, "New fluorosurfactants for stabilizing fluorocarbon oil-in-water emulsions"

**Alex Hsu**, UCSB, Mentor: Claudio Parolo; PI: Kevin Plaxco, "Improving the sensitivity of lateral flow sensors using aptamers: Monitoring of NGAL, a biomarker of kidney injuries"

**Anaiancy Ramirez**, UCSB, Mentor: Bretton Fletcher; PI: Cyrus Safinya, "The effect of Tau isoforms on microtubule stabilization"

**Andrea Ramirez**, UCSB, Mentor: Emily Wonder; PI: Cyrus Safinya, "The role of membrane hydration in PEGylated cationic lipid vectors for targeted gene delivery"

**Andy Rosales-Elias**, UCSB, Mentor: Nevena Goluvobic; PI: Chandra Krintz, "Where's the bear? - Automating wildlife image processing using IoT and edge cloud systems"

**Carolina Espinoza**, UCSB, Mentor: Brett Yurash; PI: Quyen Nguyen, "Strategies for improving triplet-triplet annihilation upconversion"

**Chase Elliott Hawes**, UCSB, Mentor: Claudio Parolo; PI: Kevin Plaxco, "Optimization of conformational-based electrochemical biosensors"

**Cristian Sharma**, UCSB, Mentor: Daniel Morse; PI: Daniel Morse, "From squid cells to lasers"

**Dolev Bluvstein**, UCSB, Mentor: Amila Ariyaratne; PI: Ania Jayich, "Imaging single spins using diamond defect"

**Elaine Bunyan**, UCSB, Mentor and PI: Eric McFarland, " H/D exchange and methane activation on solid and molten metal surfaces"

**Eric Dang**, UCSB, Mentor: Clayton Woodcock; PI: Norbert Reich, "Characterization of CcrM and its homologs"

**Gautam Bordia**, UCSB, Mentor and PI: Otger Campas, "Creating new reconfigurable materials: Biomimetic, active 2D emulsions"

**Geoffrey Chandler Bartz**, UCSB, Mentor: Emma Filippidi; Herb Waite, "Mussel-Inspired underwater acrylic adhesives"

**Helena Steffens**, UCSB, Mentor: Meghan Nichol; PI: Javier Read de Alaniz, "Aza-piancatelli rearrangement for the synthesis of cyclopentenones"

**Luis Limon**, UCSB, Mentor: James Shaum; PI: Javier Read de Alaniz, "Incorporating nitrogen functionality into small molecules through a copper catalyzed radical addition process"

**Madeline Beeson**, UCSB, Mentor: Zachariah Berkson; PI: Bradley Chmelka, "Organic-inorganic interactions in the historical pigment Maya Blue"

**Maxwell Bocheff**, UCSB, Mentor: Alicia Lund; PI: Songi Han, "Quasi-optics of EPR and NMR"

**Ngan Nguyen**, UCSB, Mentor: Emre Discekici; PI: Javier Read de Alaniz, "Endo-protected maleimide synthesis and polymerization"

**Nicholas Rommelfanger**, UCSB, Mentor and PI: Paolo Luzzatto-Fegiz, "Space-based measurements of cohesive sediment dynamics"

**Quentin Kim**, UCSB, Mentor: Ali Chamas; PI: Susannah Scott, "Synthesis of metal doped catalysts for conversion of lignin via alcoholysis and hydrogenolysis"

**Samuel Holton**, UCSB, Mentor: Alex Moreland; PI: Gui Bazan, "Designing conjugated oligoelectrolyte monolayers for increasing the power density of microbial fuel cells"

**Syrian Truong**, UCSB, Mentor and PI: Mark Srednicki, "stochastic series expansion quantum monte carlo study of the long-range transverse-field ising model in one-dimension"

**Teresa Lo**, UCSB, Mentor and PI: Deborah Fygenson, "Design and construction of three site DX-DNA nanotube tracks for the study of light-powered DNA nanomotors"

**Valerie Lensch**, UCSB, Mentor: Caitlin Sample; PI: Craig Hawker, "metal-free room temperature vulcanization and functionalization of silicones"

***RET 1 & 2 2015***
**Alena Kahn,** Santa Barbara High School
Mentors: Martin Kurnik, Gabe Quintanilla
Faculty Supervisor: Kevin Plaxco
"Protein Purification for Surface Application"

**Katelyn Standerfer,** San Marcos High School
Mentor: Jeff Self
Faculty Supervisor: Chris Bates
"Next Generation Vitrimers"

**Mark Larsen,** Malibu High School
Mentor: Naveen Venkatesan
Faculty Supervisor: Michael Chabinyc
"Charge Transport in a Two-Dimensional Hybrid-Halide Perovskite"

**Sue Squires,** Los Olivos School
Mentor: Julia Sweet
Faculty Supervisor: Uta Passow
"TEP precursor measurement"

**Elia Avalos**, Hueneme High School
Water Purification Project: Electrolysis & Renewable energy

**Erika Alstot**, Haydock Intermediate School
How can you survive on Mars?

**Robert Johnstone** Buena High School
Manufacturing Technology – Stone-age tools to 3D printing

**Susan Valle** Saint Bonaventure High School
The Busy Electron: Redox Reactions

#### (B) 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 are working with UCSB Evaluation expert

Ellie Sciaky to develop a long-term evaluation plan for our Research Experiences for Teachers program and hope to have the first results of these over the course of the coming year.

*Intern First-Author Presentations at Conferences*
SCCUR:
Abel Prieto-Flores, "Modeling the Frequency Spectrum of AM CVn Systems by Solving the Radiative Transfer Equation", Southern California Conference on Undergraduate Research, California Polytechnic University, Pomona, CA, November 18, 2017

Cristian Sharma, "From Squid Cells to Lasers", Southern California Conference on Undergraduate Research, California Polytechnic University, Pomona, CA, November 18, 2017

Anaiancy Ramirez, "The effect of Tau isoforms on microtubule stabilization", Southern California Conference on Undergraduate Research, California Polytechnic University, Pomona, CA, November 18, 2017

Catrina Wilson, "Cathodes for Next-Generation Batteries", Southern California Conference on Undergraduate Research, California Polytechnic University, Pomona, CA, November 18, 2017

SACNAS:
Catrina Wilson, "Cathodes for Next-Generation Batteries", SACNAS conference, Salt Lake City, UT, October 18-22, 2017.

Anaiancy Ramirez, "The effect of Tau isoforms on microtubule stabilization", SACNAS conference, Salt Lake City, UT, October 18-22, 2017.

WoPhys:
Jenna Ott, "Melt Electrostatic Writing (MEW) of a Human Trabecular Meshwork Scaffold", WoPhys Conference, University of Nebraska, NE, November 9-11, 2017

Sabreena Sukhram, "The Relaxation Mechanism of Indigo",WoPhys Conference, University of Nebraska, NE, November 9-11, 2017

ABRCMS:
Jaime Guerrero, "Mechanism of Contact Dependent Growth Inhibition - Interactions of an Escherichia coli Toxin with Components of the Inner Membrane", ABRMCS Conference, Phoenix, AZ, November 2-4, 2017

***Undergraduate Publications (undergraduate in bold)***

1. Barel, I., **Naughton, B**., Reich, N. O., & Brown, F. L. H. (2018). Specificity versus Processivity in the Sequential Modification of DNA: A Study of DNA Adenine Methyltransferase. *Journal of Physical Chemistry B, 122*(3), 1112-1120. doi:10.1021/acs.jpcb.7b10349
2. Bozekowski, J. D., **Graham, A. J**., & Daugherty, P. S. (2018). High-titer antibody depletion enhances discovery of diverse serum antibody specificities. *Journal of Immunological Methods, 455*, 1-9. doi:10.1016/j.jim.2018.01.003
3. Butala, M. M**., Perez, M**. A., Arnon, S., Gobel, C., Preefer, M. B., & Seshadri, R. (2017). Rapid microwave-assisted preparation of binary and ternary transition metal sulfide compounds. *Solid State*

*Sciences, 74*, 8-12. doi:10.1016/j.solidstatesciences.2017.09.010

4. Chui, M., Metzker, G., Bernt, C. M., **Tran, A. T**., Burtoloso, A. C. B., & Ford, P. C. (2017). Probing the Lignin Disassembly Pathways with Modified Catalysts Based on Cu-Doped Porous Metal Oxides. *ACS Sustainable Chemistry & Engineering, 5*(4), 3158-3169. doi:10.1021/acssuschemeng.6b02954
5. Chuong, T. T., Pallaoro, A., **Chaves, C. A**., Li, Z., Lee, J., Eisenstein, M., Soh, H. T. (2017). Dual-reporter SERS-based biomolecular assay with reduced false-positive signals. *Proceedings of the National Academy of Sciences of the United States of America, 114*(34), 9056-9061. doi:10.1073/pnas.1700317114
6. Macauley, C. A., **Fernandez, A. N**., & Levi, C. G. (2017). Phase equilibria in the ZrO2-YO1.5-TaO2.5 system at 1500 degrees C. *Journal of the European Ceramic Society, 37*(15), 4888-4901. doi:10.1016/j.jeurceramsoc.2017.06.031
7. Morales, D. P., Wonderly, W. R., Huang, X., McAdams, M., **Chron, A. B**., & Reich, N. O. (2017). Affinity-Based Assembly of Peptides on Plasmonic Nanoparticles Delivered Intracellularly with Light Activated Control. *Bioconjugate Chemistry, 28*(7), 1816-1820. doi:10.1021/acs.bioconjchem.7b00276
8. Navarrete, J., **Siefe, C**., **Alcantar, S.,** Belt, M., Stucky, G. D., & Moskovits, M. (2018). Merely Measuring the UV-Visible Spectrum of Gold Nanoparticles Can Change Their Charge State. *Nano Letters, 18*(2), 669-674. doi:10.1021/acs.nanolett.7b02592
9. Niu, J., Page, Z. A., Dolinski, N. D., Anastasaki, A., **Hsueh, A. T**., Soh, H. T., & Hawker, C. J. (2017). Rapid Visible Light-Mediated Controlled Aqueous Polymerization with In Situ Monitoring. *ACS Macro Letters, 6*(10), 1109-1113. doi:10.1021/acsmacrolett.7b00587
10. Upham, D. C., Agarwal, V., **Khechfe, A**., Snodgrass, Z. R., Gordon, M. J., Metiu, H., & McFarland, E. W. (2017). Catalytic molten metals for the direct conversion of methane to hydrogen and separable carbon. *Science, 358*(6365), 917-920. doi:10.1126/science.aao5023
11. Yoo, S. J., Evanko, B., Wang, X. F., **Romelczyk, M**., Taylor, A., Ji, X. L., Stucky, G. D. (2017). Fundamentally Addressing Bromine Storage through Reversible Solid-State Confinement in Porous Carbon Electrodes: Design of a High-Performance Dual-Redox Electrochemical Capacitor. *Journal of the American Chemical Society, 139*(29), 9985-9993. doi:10.1021/jacs.7b04603
12. Zhang, M. W., Nowak, M., de Molina, P. M., **Abramovitch, M., Santizo, K**., Mitragotri, S., & Helgeson, M. E. (2017). Synthesis of Oil-Laden Poly(ethylene glycol) Diacrylate Hydrogel Nanocapsules from Double Nanoemulsions. *Langmuir, 33*(24), 6116-6126. doi:10.1021/acs.langmuir.7b01162

## 7. POSTDOCTORAL MENTORING PLAN AND DATA MANAGEMENT PLAN

### Postdoctoral Mentoring Plan

The UCSB 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 UCSB 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 multiple perspectives provided by multiple advisors also gives postdoctoral fellows a leg up in their job searches.

In that vein, 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 UCSB MRSEC has been very successful in using alternate funding sources to award these travel fellowships.

Postdoctoral fellows are actively involved in speaking and participating in MRSEC seminars and outreach events. They are also involved in planning events, and choosing and inviting speakers to bring to campus. 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 numbers of non-MRSEC attendees who usually learn of them by word of mouth or through the UCSB Graduate Division. The student organization, Graduate Students for Diversity in Science, plays an important role in the organization and advertising of these activities. Some of the programs organized or co-organized during this reporting period include:

(i) A Career Journey Through Academia, Wednesday, October 4, 2017 by Prof. Angela Belcher, James Mason Crafts Professor, Professor of Materials Science and Engineering, and Professor of Bioengineering at Massachusetts Institute of Technology.
(ii) Non-academic Careers: John Kasianowicz, NIST, Tuesday, November 14, 2017.
(ii) Academic Careers at Community Colleges – Panel Discussion, Wednesday, November 15, 2017.

**Data Management Plan**

MRSEC research principally produces research data, in the form of lab notebooks and 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 the facility managers, researchers, PIs, and the computational facility manager. The variety and quantity of UCSB MRSEC instrumentation generates extremely diverse data types. 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, organized and maintained by the IRGs. File shares have been created for specific projects and IRGs as needed. Data are reduced and analyzed by the MRSEC researchers using dedicated workstations, personal computers, or compute clusters as appropriate. Once data has been analyzed it is returned to file shares and/or archival media specified as support for research publications.

**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 will occur primarily over the internet *via* Merritt's APIs and web interface. Very large datasets may reside on locally hosted UCSB MRSEC servers with persistent URLs. The list of MRSEC supported publications will be monitored once a year for researcher data management practices and researchers notified of best-practices and available resources. The University of California, Santa Barbara retains intellectual property rights to the data and data in support of patents may be delayed in publication until the patent is granted. Raw data resides on storage at the UCSB 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, re-distribution, and the production of derivatives:** The goal of all the UCSB-MRSEC supported research is to widely disseminate the work, with appropriate acknowledgement of the grant, in the archival journal literature. Following current practice, all publications PDF files are provided to the NSF annually, for verification of the contents, including acknowledgements. All UCSB MRSEC faculty are strongly encouraged to publish post-prints of their research (for which DOIs are already available) 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.

**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 of 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 UCSB MRSEC. Data security and integrity is of central concern to the UCSB MRSEC, and we plan to mirror data stores to UCLA in the near-term. 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.**

UCSB MRSEC leadership and members believe inclusiveness and diversity at every stakeholder level is crucial to continued success. The school populations we serve via our K-12 and RET programs are majority Hispanic, and all of the programs described in the previous section consciously engage with such a diverse community. At the undergraduate level, as befits our newly established (2015) status as an HSI, we are proud of the number of URM students who are mentored by our programs, including through our two PREM partnerships with UT El Paso and Jackson State, and an expanded NSF-LSAMP program for which we are the UCSB locus. In regard to the two PREM partnerships, we have submitted renewal proposals with both partners and eagerly await the results of the competition.

**Fig. 18.** MROP 2018: Undergraduate students and a graduate student (Glake Hill group) from Jackson State University with MRSEC Eductaion Staff Drs. Julie Standish and Dorothy Pak, during a break in the schedule.

Furthermore, we encourage URM STEM interns from UCSB, as well as from our summer internship programs to apply for graduate programs around the nation through career-building activities, potentially helping expand the pipeline. Going forward, we will work with other MRSEC centers to introduce our interns to graduate opportunities in other MRSEC programs. An example of such a partnership involves showcasing MRSEC research activities, facilities, and opportunities to the broader scientific community through event booths and symposia at national conferences such as SACNAS, and at the recent APS March Meeting. One of the guiding principles of the UCSB MRSEC is to try and integrate all stakeholders at all levels, with the different MRSEC activities. Illustrative of this is the use of the annual MROP event, described in greater detail in section 9, as a means of engaging with students from our PREM partners (Figure 18).

Increase diversity at the level of graduate students and postdoctoral fellows is an important goal of the UCSB MRSEC. With regard to URM graduate students, we are beginning to see the results of past efforts, and will build on this momentum. Summer internships, including our programs with our PREM partners, have been particularly successful in increasing the number of URM graduate students. We are closely partnering with UCSB Graduate Division Dean Carol Genetti in her newly launched campus-wide graduate diversity program, which is designed as a series of integrated resources to support students from first point of contact with the campus to recruitment, matriculation, commencement, and beyond. Student-focused programming is complemented by resources for departments and faculty. **Seshadri** and **Shea** represent Materials, and Chemistry and Biochemistry respectively, on the Graduate Dean's Advisory Board on Diversity. The student-run UCSB MRSEC organization Graduate Students for Diversity in Science (GSDS) helps to sensitize the community on the need for creating an expanded STEM pipeline at all levels, and serves the secondary role of a student/postdoctoral advisory body.

**(b) Plans for the next reporting period**

The UCSB MRSEC will continue to actively engage with diversity initiatives at every level, ranging from K–12 programs through the inclusion of new faculty investigators though Seed Programs. At the level of undergraduate and graduate students, we eagerly await the results of the PREM competition. At the postdoctoral level, we have been leveraging commitments from UCSB's Graduate Division to expanding

diversity in a manner consistent with University policy and California state law. The first successful outcomes of such efforts have taken place just outside of this reporting period and will be described in detail in the next report.

## 9. KNOWLEDGE TRANSFER TO INDUSTRY AND OTHER SECTORS

The UCSB 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 UCSB-Mitsubishi Chemical Center for Advanced Materials (now over 15 years old, led by **Fredrickson** who also coordinates all UCSB MRSEC Industrial Outreach) and the more recently formed Dow Materials Institute at UCSB (led by **Hawker**) work with the UCSB MRSEC in a number of synergistic ways, and are co-located with the UCSB 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. Dow Chemicals has also contributed to improving the laboratory safety culture of the UCSB MRSEC; a number of our students and postdoctoral associates have been trained in safety on-site in Midland Michigan, and have brought back the safety culture to UCSB. The Complex Fluids Design Consortium (most recent meeting in February 2018), an Academic-Industry-National Lab partnership that has been in existence for over 14 years, has inspired a new consortium on Soft-Matter Interfaces that aligns with proposed IRG-3 research. Annually, our industrial partners meet with UCSB MRSEC faculty, graduate students, and postdoctoral researchers at a two-day symposium, the Materials Research Outreach Program (MROP), which was held in early February 2018; this event also involves our PREM partners, and talks appropriate for a general audience are specially advertised, illustrating the integration of all stakeholders at all levels (Figure 19).

**Fig. 19(a).** MROP 2018: Graduate student Claire McLellan explaining the use of N-V centers in diamond for detecting weak currents in biological systems.

**Fig. 19(b).** MROP 2018: An animated discussion during the poster session.

The combination of fundamental research challenges with an entrepreneurial, multi-disciplinary environment has inspired MRSEC researchers to drive their research beyond traditional boundaries. The UCSB MRSEC co-sponsors the annual New Venture Competition (NVC) with the Technology Management Program at UCSB, and this has helped change the model of 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, Fluency Lighting, Milo Sensors, Next Energy, and Solution Deposition Systems, with application areas ranging from agriculture to energy efficiency to health. A focal point of outreach to industry and to researchers elsewhere, are the UCSB MRSEC Shared Experimental Facilities (SEFs) which, in conjunction with the expertise of the Technical Directors (all PhD scientists), are a unique resource that allows our industrial partners to better understand known materials, and to design new ones.

## 10. INTERNATIONAL ACTIVITIES

The UCSB 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 UCSB MRSEC around the world. In addition to the named international affiliates in the IRGs, we are continuing our partnerships with Chalmers University of Technology in Göteberg, Sweden (Figure 20), and with the Korea Advanced Institute of Science and Technology in Daejon, Korea. In addition to scientific exchanges, these efforts include undergraduate internships, and jointly-run workshops and summer schools for graduate students and postdoctoral fellows. Support for undergraduate interns, and for graduate student and postdoctoral researcher travel to partner institutions is made available on a limited basis. Details of undergraduate exchanges are presented in Section 6 of this report.

**Fig. 20.** Meeting with research parners in Göteberg, Sweden in September 2018. In the picture are the eight UCSB graduate students (third from left to right) Alexandra Bayles, Nicole Michenfelder-Schauser, Leslie Chan, Jan Garcia, Elaine Thomas, Katherine Mackie, Neils Zussblatt, and Arash Nowbahar, who attended, along with faculty member **Helgeson** (far right).

The International Affiliates of IRG-1 and IRG-3, respectively Professor Olivier Thomas (Aix Marseille Université) and Professor Fabien Barthelat (McGill University) have both respectively visited and given seminars on their research expertise, and this has helped initiate collaboration. Professor Thomas brings highly specialized synchrotron micro- and nano-diffraction tools, including *operando* techniques, to the table. Professor Barthelat researches the design fabrication and testing of novel high-performance engineering materials and systems inspired by nature, and his talk at the 2018 MROP helped introduce him to a larger audience at UCSB.

## 11. SHARED EXPERIMENTAL AND COMPUTATIONAL FACILITIES

The Shared Experimental/Computational Facilities continue to be a key focus of the UCSB MRSEC, offering state-of-the-art materials instrumentation to a wide network of university and industry partners. Maintained and operated by highly qualified technical staff, these facilities continue to offer world-class instrumentation to users locally, nationally, and internationally for the advancement of materials science. In the past year, the MRSEC has benefited from the expansion of the Materials Research Lab with the additional 2000 sq ft lab space as the facility for low temperature materials characterization. Several new pieces of sophisticated instrumentation have been added to our current capabilities. The instruments join complementary analytical techniques in near proximity to improve user accessibility. The new research space has been uniquely designed to increase our facilities' engagement with the greater UCSB community. An overview of all of the shared experimental facilities is provided below, followed by reports from the separate facilities.

| **Facility** | **Facility Director** | **Technical Directors and Staff** | **Total Users (externals are in parenthesis)** | **Total Recharged Hours (externals are in parenthesis)** |
|---|---|---|---|---|
| Computation* | Frank Brown | Dr. Paul Weakliem<br>Nathan Rogers | 236 | n/a |
| Energy | Michael Chabinyc | Dr. Rachel Behrens | 20 | na |
| Microscopy | Daniel Gianola | Dr. Tom Mates<br>Dr. Aidan Taylor<br>Mark Cornish | 193 (23) | 4,524 (565) |
| Polymer | Craig Hawker | Dr. Rachel Behrens | 69 (10) | 892 (156) |
| Spectroscopy | Songi Han | Dr. Jerry Hu<br>Jaya Nolt<br>Shamon Walker | 163 (24) | 13,383 (2065) |
| TEMPO** | Ram Seshadri | Dr. Amanda Strom<br>Burton Sickler | 106 (12) | 5,893 (291) |
| Terahertz*** | Mark Sherwin | Dr. Nikolay Agladze | 11 (3) | 340 (75) |
| X-Ray | Cyrus Safinya | Dr. Youli Li<br>Miguel Zepeda<br>Phillip Kohl | 313 (21) | 2,464 (707) |
| Totals | | | 1,111(93) | 27,496 (3,859 ) |

* Partnered with the California NanoSystems Institute under the rubric Center for Scientific Computing
** TEMPO = **T**hermal **E**lectronic/**E**lemental **M**agnetic **P**orosity, and **O**ptical
*** Partner facility run by the Institute for Terahertz Science and Technology

**Computation:** The MRSECs Computational Facility continues to be co-located and operated synergistically with the California NanoSystems Institute (CNSI) in the Center for Scientific Computing (CSC) (Directors: Prof. Frank Brown, Dr. Paul Weakliem, Nathan Rogers). The CSC served 230 plus users affiliated with over 30 research groups and 91 faculty members. Additionally, several computationally oriented courses utilized CSC clusters for short terms. Through the reporting period, CSC cluster users have utilized more than 5 million hours of aggregate CPU time. The CSC continued its broad campus impact by reaching out to UCSB graduate students and educating them on available campus HPC and XSEDE resources. In

addition, the CSC held beginning of the year workshops on *Using Singularity Containers on HPC Resources*, *Using Python for Scientific Computing*, *Using MatLab and R on HPC Resources*, and *XSEDE Access and Information* in addition to *Basic Linux Instruction for HPC*. MRSEC funds were used to augment the GPU nodes for the MRSEC condo cluster and to transition the condo filesystem to a high performance BeeGFS filesystem. GPU nodes are heavily used in both IRG-2 and IRG-3 for polymeric DFT simulations.

**Energy:** The Energy Facility (*Director:* Prof. **Michael Chabinyc**; *Lab Manager:* Dr. Rachel Behrens) continues to expand and develop its capabilities for current and future users. The Energy Facility currently serves 3 groups in 2 departments and one local start-up company with approximately 900 overall usage hours.

**Microscopy and Microanalysis Facility**: (*Director:* Prof. **Daniel Gianola**; *Lab Managers:* Mark Cornish, Dr. Aidan Taylor, Dr. Tom Mates) This facility provides a range of advanced methods for the analysis of both hard and soft materials. Over the last reporting period, this facility served a total of 50 groups on campus. Over this period two new SEMs with a broader range of features, better resolution and more user-friendly interfaces have been acquired.

**Polymer:** The Polymer Characterization Facility (*Director:* Prof. **Craig Hawker**; *Lab Manager:* Dr. Rachel Behrens) continues to focus on streamlining current processes to optimize efficiency, reproducibility, and accuracy while expanding its analytical capabilities to serve its 170 trained internal and external users. Currently, the Polymer Facility serves 18 UCSB research groups in 6 departments and 10 off-campus users from both academia and industry. In the past year, the Polymer Characterization Facility has worked with 2 new industrial, 3 new academic contacts, continues work with 5 previously-associated companies and universities, and a 5-year collaboration with the FDA.

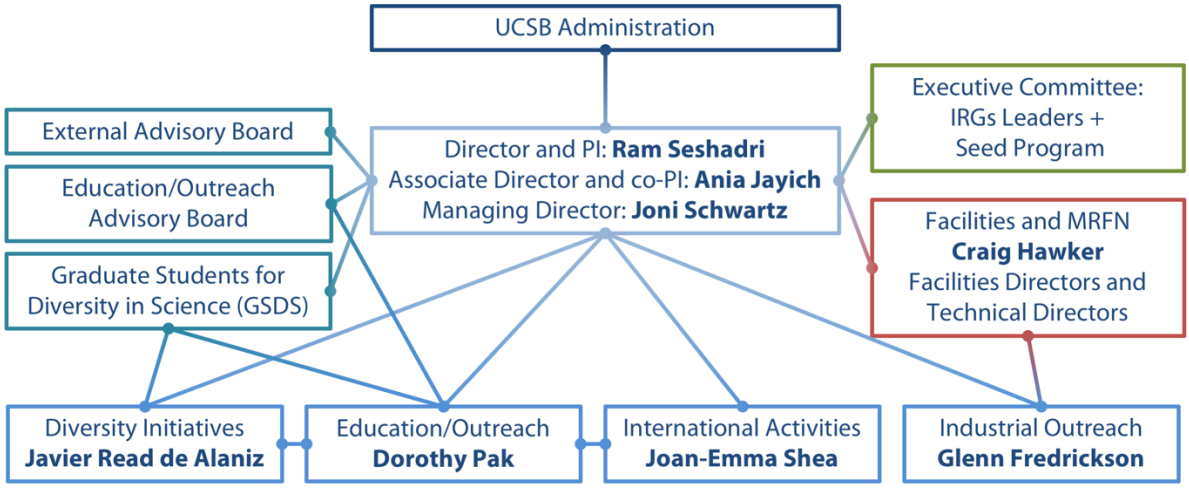
**Spectroscopy:** As a state-of-the-art shared magnetic resonance laboratory, the Spectroscopy Facility (*Director:* Prof. **Songi Han**; *Lab Manager:* Dr. Jerry Hu) continues to perform at a very high level. During the current period, a total number of 163 users (of which 24 were external, accounting for 15%) benefited from various advanced spectroscopy capabilities of the facility. 13,383 total recharge hours were recorded, of which 15% was external (or 2065 recharge hours), showcasing the standing and need of the shared Spectroscopy Facility beyond that of the UCSB campus.

**TEMPO:** The TEMPO (Thermal Electronic/Elemental Magnetic Porosity Optical) facility (*Director:* Prof. **Ram Seshadri**; *Lab Manager:* Dr. Amanda Strom) is a shared facility with over 106 on-campus users from more than 30 different groups and 8 different departments or organizations. The facility also served 16 off-campus active users from academia and local industry in addition to accepting samples from external users for analysis by TEMPO staff. Last year's expansion of the Low-Temperature Characterization Facility has allowed for several new pieces of equipment to come into the lab including a new cryogen-free milli-K system from Oxford with a 14 T magnet.

**X-Ray:** During the current period, the X-Ray Facility (*Director:* Prof. Cyrus Safinya; *Lab Manager:* Dr. Youli Li) served a total of 334 active users with 3171 recharge hours (78% internal, 22% external). This facility operates both commercial and custom developed x-ray diffractometers used by this user base. To further its characterization capability, in the 2017 to 2018 time period, the facility carried out internal development to upgrade the SAXS-WAXS instrument with enhanced data collection and analysis software.

## 12 ADMINISTRATION AND MANAGEMENT

The management structure, as depicted in the organizational chart shown below includes new leadership (PI and Director **Seshadri** and Co-PI and Associate Director **Jayich**), who report to the Dean of Engineering at UCSB. The Dean in turn works in close consultation with the Dean of Science, and the Vice Chancellor for Research to ensure the success of the MRSEC. **Hawker** l now serve as the coordinator of the SEFs. **Fredrickson**, **Pak**, **Read de Alaniz**, and **Shea** are the other senior investigators who comprise the overall leadership team, with responsibilities as listed. The relationships between the main components of the UCSB 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 seven new 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 Luis Echegoyen, who also directs the PREM at UT El Paso, is retained from the previous board. All other members started in late 2015, played a key role in IRG selection, and have been involved in making the decision with regard to awarding Seed grants.




Management Structure. The eight-member External Advisory Board (EAB) has been newly reconstituted. The new Education/Outreach Advisory Board has members from UCSB and local schools. GSDS is a student-run organization with a focus on expanding diversity, and also serves as the student body advising the UCSB MRSEC leadership.

The IRGs are individually managed by the Co-Leaders. All individual IRGs meet once every week. The Materials Research Outreach Program (MROP) held in early February 2018 served as the annual meeting of the entire MRSEC. 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 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. The newly formed nine-member Education/Outreach Advisory Board meets with **Pak** and **Seshadri** once a year, and provides valuable guidance on a range of issues.

## 13. PLACEMENTS: STUDENTS & POSTDOCTORAL SCHOLARS

### Graduate Student Placements 2017/18

| | | |
|---|---|---|
| Barnes, Ryan | PhD | Flir Thermal Imaging Systems |
| Carpenter, Corinne* | PhD | Industry (TBD) |
| Decolvenaere, Elizabeth* | PhD | D. E. Shaw Research |
| Jenkins, Alec | PhD | N/A |
| McDearmon, Brenden | PhD | N/A |
| Melker, Anna* | PhD | Church & Dwight Co., Inc. |
| Myers, Brian | PhD | Intel Corporation |
| Santosh, Raghavan | PhD | MaxLinear, San Diego |
| Schrader, Alex | PhD | Industry (TBD) |
| Wilhelm, Menaka* | MS | NPR (science journalism) |

### Postdoctoral Scholar Placements 2017/18

| | |
|---|---|
| Bartels, Joshua | W. L. Gore & Associates |
| Kaminker, Ilia | Tel Aviv University |
| Khadilkar, Mihir | University of Mainz, Germany |
| Knight, Abigail* | University of North Carolina |
| Lawrence, Jimmy | Louisiana State University |
| Lee, In-Hwan | Ajou University |
| Lee, SangHo | Research Center for Green Fine Chemicals, Korea Research Institute of Chemical Technology |
| Liu, Yi-Xin | Academic Institution (TBD) |
| Pelliccione, Matt | Hughes Research Labs |
| Ren, Jing | Dow Electronics |
| Sanoja, Gabriel** | École supérieure de physique et de chimie industrielles (ESPCI) |
| Tree, Doug | Brigham Young University |
| Weston, Leigh | Lawrence Berkeley National Laboratory |
| Willenbacher, Johannes | BASF |

* Female

** Underrepresented Minority

## 14. LIST OF MRSEC-SUPPORTED PUBLICATIONS, SEPTEMBER 1, 2017 TO FEBRUARY 28, 2018 [ Total 33]

**IRG-1 [2]**

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

1. E. Decolvenaere, M. Gordon, R. **Seshadri**, A. **Van der Ven**, "First-principles investigation of competing magnetic interactions in (Mn,Fe) $Ru_2Sn$ Heusler solid solutions," *Phys. Rev. B* **96** (2017) 165109. DOI: 10.1103/PhysRevB.96.165109
2. E.E. Levin, J.D. Bocarsly, K.E. Wyckoff, T.M. **Pollock**, R. **Seshadri**, "Tuning the magnetocaloric response in half-Heusler/Heusler $MnNi_{1+x}Sb$ solid solutions," *Phys. Rev. Mater.* **1** (2017) 075003. DOI: 10.1103/PhysRevMaterials.1.075003

**b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256**

None

**IRG-2 [3]**

**a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [3]**

3. J. Bartels, G.E. Sanoja, C.M. Evans, R.A. **Segalman**, M.E. **Helgeson**, "Decoupling mechanical and conductive dynamics of polymeric ionic liquids via a trivalent anion additive," *Macromolecules* **50** (2017) 8979-8987. DOI: 10.1021/acs.macromol.7b01351
4. I.-H. Lee, E.H. Discekici, S.L. Shankel, A. Anastasaki, J. **Read de Alaniz**, C.J. **Hawker**, D.J. Lunn, "Desulfurization–bromination: Direct chain-end modification of RAFT polymers," *Polym. Chem*. **8** (2017) 7188-7194. DOI: 10.1039/C7PY01702B
5. J.M. Ren, J. Lawrence, A.S. Knight, A. Abdilla, R. Bou Zerdan, A.E. Levi, B. Oschmann, W.R. Gutekunst, S.-H. Lee, Y. Li, A.J. McGrath, C.M. **Bates**, G.G. Qiao, C.J. **Hawker**, "Controlled formation and binding selectivity of discrete oligo(methyl methacrylate) stereocomplexes," *J. Am. Chem. Soc.* **140** (2018) 1945-1951. DOI: 10.1021/jacs.7b13095

**b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256**

None

**IRG-3 [2]**

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

6. I. Kaminker, W. Wei, A.M. Schrader, Y. Talmon, M.T. **Valentine**, J.N. Israelachvili, J.H. **Waite**, S. **Han**, "Simple peptide coacervates adapted for rapid pressure-sensitive wet adhesion," *Soft Matter* **13** (2017) 9122-9131. DOI: 10.1039/C7SM01915G
7. A.S. Knight, J. Larsson, J.M. Ren, R. Bou Zerdan, S. Seguin, R. Vrahas, J. Liu, G. Ren, C.J. **Hawker**, "Control of amphiphile self-assembly via bioinspired metal ion coordination," *J. Am. Chem. Soc.* **140** (2018) 1409-1414. DOI: 10.1021/jacs.7b11005

**b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256**

None

**SEED**

**a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256**

None

**b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256**

None

**SHARED FACILITIES [26]**


8. N.L. Adamski, Z. Zhu, D. Wickramaratne, C.G. **Van de Walle**, "Hybrid functional study of native point defects and impurities in $ZnGeN_2$," *J. Appl. Phys*. **122** (2017) 195701. DOI: 10.1063/1.4999790
9. G.C.B. Alexander, D.H. Fabini, R. **Seshadri**, M.G. Kanatzidis, "$AuPb_2I_7$: A narrow bandgap $Au^{3+}$ iodide semiconductor," *Inorg. Chem.* **57** (2018) 804-810. DOI: 10.1021/acs.inorgchem.7b02723
10. R. Barnes, S. Sun, Y. Fichou, F.W. Dahlquist, M. Heyden, S. **Han**, "Spatially heterogeneous surface water diffusivity around structured protein surfaces at equilibrium," *J. Am. Chem. Soc*. **139** (2017) 17890-17901. DOI: 10.1021/jacs.7b08606
11. J.S. Bechtel, A. **Van der Ven**, "Octahedral tilting instabilities in inorganic halide perovskites," *Phys. Rev. Mater.* **2** (2018) 025401. DOI: 10.1103/PhysRevMaterials.2.025401
12. M.F. Carilli, K.T. Delaney, G.H. **Fredrickson**, "Nucleation of the lamellar phase from the disordered phase of the renormalized Landau-Brazovskii model," *J. Chem. Phys.* **148** (2018) 054903. DOI: 10.1063/1.5003150
13. W. Cheng, N. Singh, W. Elliott, J. Lee, A. Rassoolkhani, X. Jin, E. W. McFarland, S. Mubeen, "Earth-abundant tin sulfide-based photocathodes for solar hydrogen production," *Adv. Sci*. **5** (2018) 1700362. DOI: 10.1002/advs.201700362
14. C. Cozzan, G. Lheureux, N. O'Dea, E.E. Levin, J. Graser, T.D. Sparks, S. Nakamura, S.P. DenBaars, C. Weisbuch, R. **Seshadri**, "Stable, heat-conducting phosphor composites for high-power laser lighting," *ACS Appl. Mater. Interfaces* **10** (2018) 5673-5681. DOI: 10.1021/acsami.8b00074
15. S.P.O. Danielsen, G.E. Sanoja, S.R. McCuskey, B. Hammouda, G.C. Bazan, G.H. **Fredrickson**, R.A. **Segalman**, "Mixed conductive soft solids by electrostatically driven network formation of a conjugated polyelectrolyte," *Chem. Mater.* **30** (2018) 1417-1426. DOI: 10.1021/acs.chemmater.7b05303
16. D.H. Fabini, T.A. Siaw, C.C. Stoumpos, G. Laurita, D. Olds, K. Page, J.G. Hu, M.G. Kanatzidis, S. **Han**, R. **Seshadri**, "Universal dynamics of molecular reorientation in hybrid lead iodide perovskites," *J. Am. Chem. Soc.* **139** (2017) 16875-16884. DOI: 10.1021/jacs.7b09536
17. P. Ganguly, P. Boserman, N.F.A. van der Vegt, J.-E. **Shea**, "Trimethylamine *n*-oxide counteracts urea denaturation by inhibiting protein-urea preferential interaction," *J. Am. Chem. Soc*. **140** (2018) 483-492. DOI: 10.1021/jacs.7b11695
18. M. Goyal, L. Galletti, S. Salmani-Rezaie, T. Schumann, D.A. Kealhofer, S. Stemmer, "Thickness dependence of the quantum Hall effect in films of the three-dimensional Dirac semimetal $Cd_3As_2$," *APL Mater.* **6** (2018) 026105. DOI: 10.1063/1.5016866

19. J.H. Grebenkemper, J.D. Bocarsly, E.E. Levin, G. Seward, C. Heikes, C. Brown, S. Misra, F. Seeler, K. Schierle-Arndt, S.D. **Wilson**, R. **Seshadri**, "Rapid microwave preparation and composition tuning of the high-performance magnetocalorics $(Mn,Fe)_2(P,Si)$," *ACS Appl. Mater. Interfaces* **10** (2018) 7208-7213. DOI: 10.1021/acsami.7b16988
20. Y. Kang, H. Peelaers, K. Krishnaswamy, C.G. **Van de Walle**, "First-principles study of direct and indirect optical absorption in $BaSnO_3$," *Appl. Phys. Lett.* **112** (2018) 062106. DOI: 10.1063/1.5013641
21. N. Khalid, M. Hussain, H.S. Young, M. Ashraf, M. Hameed, R. Ahmad, "Lead concentrations in soils and some wild plant species along two busy roads in Pakistan," *Bull. Environ. Contam. Toxicol*. **100** (2018) 250-258. DOI: 10.1007/s00128-017-2247-7
22. E. Lim, K.A. Peterson, G.M. Su, M.L. **Chabinyc**, "Thermoelectric properties of poly(3-hexylthiophene) (P3HT) doped with 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane ($F_4$TCNQ) by vapor-phase infiltration," *Chem. Mater.* **30** (2018) 998-1010. DOI: 10.1021/acs.chemmater.7b04849
23. J. Navarrete, C. Siefe, S. Alcantar, M. Belt, G.D. Stucky, M. Moskovits, "Merely measuring the UV–visible spectrum of gold nanoparticles can change their charge state," *Nano Lett.* **18** (2018) 669-674. DOI: 10.1021/acs.nanolett.7b02592
24. R. Nery-Azevedo, A. Banerjee, T.M. **Squires**, "Diffusiophoresis in ionic surfactant gradients," *Langmuir* **33** (2017) 9694-9702. DOI: 10.1021/acs.langmuir.7b01094
25. D.L. Poerschke, J.H. Shaw, N. Verma, F.W. Zok, C.G. Levi, "Interaction of yttrium disilicate environmental barrier coatings with calcium-magnesium-iron alumino-silicate melts," *Acta Mater.* **145** (2018) 451-461. DOI: 10.1016/j.actamat.2017.12.004
26. M.B. Preefer, B. Oschmann, C. J. **Hawker**, R. **Seshadri**, F. Wudl, "High sulfur content material with stable cycling in lithium-sulfur batteries," *Angew. Chem. Int. Ed*. **56** (2017) 15118-15122. DOI: 10.1002/anie.201708746
27. E.C. Schueller, G. Laurita, D.H. Fabini, C.C. Stoumpos, M.G. Kanatzidis, R. **Seshadri**, "Crystal structure evolution and notable thermal expansion in hybrid perovskites formamidinium tin iodide and formamidinium lead bromide," *Inorg. Chem.* **57** (2018) 695-701. DOI: 10.1021/acs.inorgchem.7b02576
28. T. Schumann, L. Galletti, D.A. Kealhofer, H. Kim, M. Goyal, S. Stemmer, "Observation of the quantum hall effect in confined films of the three-dimensional Dirac semimetal $Cd_3As_2$," *Phys. Rev. Lett.* **120** (2018) 016801. DOI: 10.1103/PhysRevLett.120.016801
29. S. Smeets, Z.J. Berkson, D. Xie, S.I. Zones, W. Wan, X. Zou, M.-F. Hsieh, B.F. **Chmelka**, L.B. McCusker, C. Baerlocher, "Well-defined silanols in the structure of the calcined high-silica zeolite SSZ-70: New understanding of a successful catalytic material," *J. Am. Chem. Soc*. **139** (2017) 16803-16812. DOI: 10.1021/jacs.7b08810
30. D.C. Upham, V. Agarwal, A. Khechfe, Z.R. Snodgrass, M.J. Gordon, H. Metiu, E.W. McFarland, "Catalytic molten metals for the direct conversion of methane to hydrogen and separable carbon," *Science* **358** (2017) 917-921. DOI: 10.1126/science.aao5023
31. N.R. Venkatesan, J.G. Labram, M.L. **Chabinyc**, "Charge-carrier dynamics and crystalline texture of layered Ruddlesden–Popper hybrid lead iodide perovskite thin films," *ACS Energy Lett.* **3** (2018) 380-386. DOI: 10.1021/acsenergylett.7b01245
32. W. Wang; H. Peelaers; J.-X. Shen; A. Janotti; C.G. **Van de Walle**, "First-principles characterization of defects in $WO_3$," *Proceedings* Vol. **10533**, *Oxide-based Materials and Devices IX*; 105332C (2018). Event: SPIE OPTO, 2018, San Francisco, CA. DOI: 10.1117/12.2303688
33. M. Zhang, P.T. Corona, N. Ruocco, D. Alvarez, P. Malo de Molina, S. Mitragotri, M.E. **Helgeson**, "Controlling complex nanoemulsion morphology using asymmetric cosurfactants for the preparation of polymer nanocapsules," *Langmuir* **34** (2018) 978-990. DOI: 10.1021/acs.langmuir.7b02843

## PATENTS BY MRSEC-SUPPORTED FACULTY, DMR 1720256, 2017-2018

**(a) Patents granted during the current period**

"Nanostructured layers of thermoelectric materials"
M.L. **Chabinyc**, J.J. Urban, J. Lynch, N. Coates, J.D. Forster, A. Salu, B. Russ
U.S. Patent 9,882,108 (January 30, 2018)

"Copolymer formulation for directed self-assembly, methods of manufacture thereof and articles comprising the same"
G.H. **Fredrickson**, B. Kim, P. Trefonas, V. Ginzburg, P. Hustad
U.S. Patent 9,765,214 (September 19, 2017), U.S. Patent 9,772,554 (September 26, 2017), and U.S. Patent 9,840,637 (December 12, 2017)

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

"Colorimetric sensors and methods of using colorimetric sensors"
J. **Read de Alaniz**, C.J. **Hawker**. T. Margalith, J. Hemmer, Y. Diaz, A.S. Knight, N.J. Treat, Z.A. Page
U.S. Patent Application No. PCT/US17/57400 filed 10/19/17.

**(c) Patents licensed during the current period**

None

## 15. BIOSKETCHES OF NEW INVESTIGATORS ADDED

**John Harter**
Materials Department, University of California, Santa Barbara, CA 93106-5050
Phone: (805) 893-3706 • Email: harter@ucsb.edu • Web: https://labs.materials.ucsb.edu/harter/john/

**(a) Professional Preparation**

| Institution | Major or Area | Degree and Year |
|---|---|---|
| University of Florida, Gainesville, FL, USA | Physics, Mathematics | B.Sc. 2006 |
| Cornell University, Ithaca, NY, USA | Physics | Ph.D. 2013 |
| California Institute of Technology, Pasadena, CA, USA | Physics | Postdoc. 2014-2017 |

**(b) Appointments**

| Institution | Position | Years |
|---|---|---|
| Materials Department, University of California, Santa Barbara, CA, USA | Assistant Professor | 2017-present |

**(c) Products i: Five products most closely related to the project:**

1. J. W. Harter, Z. Y. Zhao, J.-Q. Yan, D. G. Mandrus, D. Hsieh, A parity-breaking electronic nematic phase transition in the spin-orbit coupled metal $Cd_2Re_2O_7$, *Science* **356**, 295-299 (2017). DOI: 10.1126/science.aad1188
2. J. W. Harter, H. Chu, S. Jiang, N. Ni, D. Hsieh, Nonlinear and time-resolved optical study of the 112-type iron-based superconductor parent $Ca_{1-x}La_xFeAs_2$ across its structural phase transition, *Phys. Rev. B* **93**, 104506 (2016). DOI: 10.1103/PhysRevB.93.104506
3. J. W. Harter, L. Niu, A. J. Woss, D. Hsieh, High-speed measurement of rotational anisotropy nonlinear optical harmonic generation using position-sensitive detection, *Opt. Lett.* **40**, 4671 (2015). DOI: 10.1364/OL.40.004671
4. J. W. Harter, L. Maritato, D. E. Shai, E. J. Monkman, Y. Nie, D. G. Schlom, K. M. Shen, Nodeless superconducting phase arising from a strong ($\pi$, $\pi$) antiferromagnetic phase in the infinite-layer electron-doped $Sr_{1-x}La_xCuO_2$ compound, *Phys. Rev. Lett.* **109**, 267001 (2012). DOI: 10.1103/PhysRevLett.109.267001
5. J. W. Harter, L. Maritato, D. E. Shai, E. J. Monkman, Y. Nie, D. G. Schlom, K. M. Shen, Doping evolution and polar surface reconstruction of the infinite-layer cuprate $Sr_{1-x}La_xCuO_2$, *Phys. Rev. B* **92**, 035149 (2015). DOI: 10.1103/PhysRevB.92.035149

**(c) Products ii: Five other significant products:**

1. J. W. Harter, D. M. Kennes, H. Chu, A. de la Torre, Z. Y. Zhao, J.-Q. Yan, D. G. Mandrus, A. J. Millis, D. Hsieh, Evidence of an improper displacive phase transition in $Cd_2Re_2O_7$ via time-resolved coherent phonon spectroscopy, *Phys. Rev. Lett.* **120**, 047601 (2018). DOI: 10.1103/PhysRevLett.120.047601
2. J. W. Harter, B. M. Andersen, J. Bobroff, M. Gabay, P. J. Hirschfeld, Antiferromagnetic correlations and impurity broadening of NMR linewidths in cuprate superconductors, *Phys. Rev. B* **75**, 054520 (2007). DOI: 10.1103/PhysRevB.75.054520
3. E. J. Monkman, C. Adamo, J. A. Mundy, D. E. Shai, J. W. Harter, D. W. Shen, B. Burganov, D. A. Muller, D. G. Schlom, K. M. Shen, Quantum many-body interactions in digital oxide superlattices, *Nat. Mater.* **11**, 855 (2012). DOI: 10.1038/nmat3405

4. S. Chatterjee, J. Trinckauf, T. Hanke, D. E. Shai, J. W. Harter, J. T. Williams, G. M. Luke, K. M. Shen, J. Geck, Formation of the coherent heavy fermion liquid at the hidden order transition in $URu_2Si_2$, *Phys. Rev. Lett.* **110**, 186401 (2013). DOI: 10.1103/PhysRevLett.110.186401
5. D. E. Shai, C. Adamo, D. W. Shen, C. M. Brooks, J. W. Harter, E. J. Monkman, B. Burganov, D. G. Schlom, K. M. Shen, Quasiparticle mass enhancement and temperature dependence of the electronic structure of ferromagnetic $SrRuO_3$ thin films, *Phys. Rev. Lett.* **110**, 087004 (2013). DOI: 10.1103/PhysRevLett.110.087004

**(d) Synergistic Activities**

1. Member of the American Physical Society (2009-present)
2. Guest lecturer for Pasadena High School physics outreach program (2015)
3. Served as DOE Office of Science peer reviewer (2018-present)

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**Kunal Mukherjee**
Materials Department, University of California, Santa Barbara CA 93106-5050
Email: kunalm@engineering.ucsb.edu + web: http://www.engr.ucsb.edu/~kunalm

**(a) Professional Preparation:**

| Institution | Major or Area | Degree and Year |
|---|---|---|
| Nanyang Technological University, Singapore | Electrical Engineering | BEng 2007 |
| Massachusetts Institute of Technology, USA | Materials Science | PhD 2014 |
| Massachusetts Institute of Technology, USA | Materials Science | Postdoc. 2014-2015 |
| IBM T.J. Watson Research Center, USA | Materials Science | Postdoc. 2015-2016 |

**(b) Appointments:**

| Institution | Position | Years |
|---|---|---|
| Materials Department, Univ. of California Santa Barbara | Asst. Professor | 2016-present |

**(c) Products i: Five publications relevant to the project:**

[1] K. Mukherjee, B.A. Wacaser, S.W. Bedell, D.K. Sadana, Rapid imaging of misfit dislocations in SiGe/Si in cross-section and through oxide layers using electron channeling contrast, Appl. Phys. Lett. 110 (2017) 232101. doi:10.1063/1.4984210.
[2] K. Mukherjee, D.A. Beaton, T. Christian, E.J. Jones, K. Alberi, A. Mascarenhas, M.T. Bulsara, E.A. Fitzgerald, Growth, microstructure, and luminescent properties of direct-bandgap InAlP on relaxed InGaAs on GaAs substrates, J. Appl. Phys. 113 (2013) 183518-183518–8. doi:10.1063/1.4804264.
[3] K. Mukherjee, D.A. Beaton, A. Mascarenhas, M.T. Bulsara, E.A. Fitzgerald, Effects of dislocation strain on the epitaxy of lattice-mismatched AlGaInP layers, J. Cryst. Growth. 392 (2014) 74–80. doi:10.1016/j.jcrysgro.2014.01.058.
[4] K. Mukherjee, A.G. Norman, A.J. Akey, T. Buonassisi, E.A. Fitzgerald, Spontaneous lateral phase separation of AlInP during thin film growth and its effect on luminescence, J. Appl. Phys. 118 (2015) 115306. doi:10.1063/1.4930990.
[5] M. Vaisman, K. Mukherjee, T. Masuda, K. Nay Yaung, E.A. Fitzgerald, M.L. Lee, Direct-Gap 2.1-2.2 eV AlInP Solar Cells on GaInAs/GaAs Metamorphic Buffers, IEEE J. Photovolt. PP (2015) 1–7. doi:10.1109/JPHOTOV.2015.2506401.

**(d) Products ii: Five other publications:**

[1] K. Mukherjee, Y. Hayamizu, C.S. Kim, L.M. Kolchina, G.N. Mazo, S.Y. Istomin, S.R. Bishop, H.L. Tuller, Praseodymium Cuprate Thin Film Cathodes for Intermediate Temperature Solid Oxide Fuel Cells: Roles of Doping, Orientation, and Crystal Structure, ACS Appl. Mater. Interfaces. 8 (2016) 34295–34302. doi:10.1021/acsami.6b08977.

[2] K. Mukherjee, P.B. Deotare, E.A. Fitzgerald, Improved photoluminescence characteristics of order-disorder AlGaInP quantum wells at room and elevated temperatures, Appl. Phys. Lett. 106 (2015) 142109. doi:10.1063/1.4917254.

[3] T.M. Christian, D.A. Beaton, K. Mukherjee, K. Alberi, E.A. Fitzgerald, A. Mascarenhas, Amber-green light-emitting diodes using order-disorder AlxIn1−xP heterostructures, J. Appl. Phys. 114 (2013) 074505. doi:10.1063/1.4818477.

[4] D.A. Beaton, T. Christian, K. Alberi, A. Mascarenhas, K. Mukherjee, E.A. Fitzgerald, Determination of the direct to indirect bandgap transition composition in AlxIn1−xP, J. Appl. Phys. 114 (2013) 203504. doi:10.1063/1.4833540.

[5] K. Mukherjee, T.-H. Teng, R. Jose, S. Ramakrishna, Electron transport in electrospun TiO2 nanofiber dye-sensitized solar cells, Appl. Phys. Lett. 95 (2009) 012101. doi:10.1063/1.3167298

**(e) Synergistic activities:**

**2017–present:** IEEE Photonics Conference Photonic Materials and Metamaterials Sub-Committee.

**2017-2018:** Invited Organizer, Electronic Materials Conference (MRS).

**Reviewer for journals:** Journal of Applied Physics, Journal of Crystal Growth, Journal of the American Ceramics Society, IEEE Journal of Photovoltaics, Nanoscale, Solar Energy Materials and Solar cells.

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**Chris G. Van de Walle**

Materials Department, University of California, Santa Barbara, CA 93106-5050

Phone: (805) 893-7144 E-mail: vandewalle@mrl.ucsb.edu http://www.mrl.ucsb.edu/~vandewalle/

**(a) Professional Preparation**

| Institution | Major or Area | Degree and Year |
|---|---|---|
| Rijksuniversiteit Gent, Belgium | Electronics | Engineer, 1982 |
| Stanford University, Stanford, CA, USA | Electrical Engineering | Ph.D., 1986 |
| IBM Research Division, Yorktown Heights, NY, USA | Physical Sciences | Postdoc, 1986-1988 |

**(b) Appointments**

| Institution | Position | Years |
|---|---|---|
| Materials Department, University of California, Santa Barbara, CA, USA | Distinguished Professor and Herbert Kroemer Chair | 2004-present |
| Xerox Palo Alto Research Center, Palo Alto, CA, USA | Principal Scientist | 1991-2004 |
| Philips Laboratories, Briarcliff Manor, NY, USA | Sr. Mbr. of Research Staff | 1988-1991 |

**(c) Products i: 5 publications relevant to the proposal (total over 400):**

1. "Hole polarons and p-type doping in boron nitride polymorphs", L. Weston, D. Wickramaratne, and C. G. Van de Walle, Phys. Rev. B **96**, 100102(R) (2017).
2. "Defects in AlN as candidates for solid-state qubits", J. B. Varley, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **93**, 161201 (2016).
3. "Defects as qubits in 3C- and 4H-SiC", L. Gordon, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **92**, 045208 (2015).
4. "Defects in SiC for quantum computing", J. R. Weber, W. F. Koehl, J. B. Varley, A. Janotti, B. B. Buckley, C. G. Van de Walle, and D. D. Awschalom, J. Appl. Phys. **109**, 102417 (2011).
5. "Quantum Computing with Defects", J. R. Weber, W. F. Koehl, J. B. Varley, A. Janotti, B. B. Buckley, C. G. Van de Walle & D. D. Awschalom, Proc. Nat. Acad. Sci. **107**, 8513 (2010).

**(c) Products ii: Five other significant products**

1. "Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors", A. Alkauskas, C. E. Dreyer, J. L. Lyons, and C. G. Van de Walle, Phys. Rev. B **93**, 201304(R) (2016).
2. "Gallium vacancy complexes as a cause of Shockley-Read-Hall recombination in III-nitride light emitters", C. E. Dreyer, A. Alkauskas, J. L. Lyons, J. S. Speck, C. G. Van de Walle, Appl. Phys. Lett. **108**, 141101 (2016).
3. "Computationally predicted energies and properties of defects in GaN", J. L. Lyons and C. G. Van de Walle, NPJ Comput. Mater. **3**, 12 (2017).
4. "First-principles theory of the luminescence lineshape for the triplet transition in diamond NV centres", A. Alkauskas, B. B. Buckley, D. D. Awschalom, and C. G. Van de Walle, New J. Phys. **16**, 073026 (2014).
5. "First-principles calculations for point defects in solids", C. Freysoldt, T. Hickel, J. Neugebauer, G. Kresse, A. Janotti, and C. G. Van de Walle, Rev. Mod. Phys. **86**, 253 (2014).

**(d) Synergistic Activities**

- Chair of three international conferences; Program Chair for the *International Conference on the Physics of Semiconductors*, Flagstaff, AZ, July 26-30, 2004.
- Member, National Academy of Engineering, 2016
- 23 patents; several patents pending.

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**Cenke Xu**
Physics Department, University of California, Santa Barbara, CA 93106-9530
Phone: (805) 893-4029 • Email: xucenke@physics.ucsb.edu

**(a) Professional Preparation**

| Institution | Major or Area | Degree and Year |
|---|---|---|
| Tsinghua University, Beijing, P. R. China | Physics | B.Sc. 2003 |
| University of California, Berkeley | Physics | Ph.D. 2007 |
| Harvard University | Physics | Postdoc. 2007-2010 |

**(b) Appointments**

| Institution | Position | Years |
|---|---|---|
| Physics Department, University of California, Santa Barbara, CA, USA | Assistant Professor | 2010-2014 |
| Physics Department, University of California, Santa Barbara, CA, USA | Associate Professor | 2014-present |

**(c) Products i: Five products most closely related to the project:**

1. Cenke Xu and S. Sachdev, Majorana liquids: the complete fractionalization of the electron, Phys. Rev. Lett. 105, 057201
2. Cenke Xu, M. Muller and S. Sachdev, . Ising and Spin orders in the iron-based Superconductors, Phys. Rev. B 78, 020501R
3. Yang Qi and Cenke Xu, Global phase diagram for Magnetism and Lattice Distortion of Fe-pnictide materials, Phys. Rev. B, 80, 094402
4. Max A. Metlitski, Ashvin Vishwanath, Cenke Xu, Duality and bosonization of (2+1)d, Phys. Rev. B 95, 205137
5. Jiangping Hu, Cenke Xu, Nematic orders in Iron-based superconductors (review), Physica C: Superconductivity, 481, 1

**(c) Products ii: Five other significant products**

1. Yi-Zhuang You, Yin-Chen He, Cenke Xu, and Ashvin Vishwanath, Symmetric Fermion Mass Generation and Deconfined Quantum Criticality, Phys. Rev. X 8, 011026
2. Chong Wang, Adam Nahum, Max A. Metlitski, Cenke Xu, T. Senthil, Deconfined quantum critical points: symmetries and dualities, Phys. Rev. X 7, 031052
3. Yan Qi Qin, Yuan-Yao He, Yi-Zhuang You, Zhong-Yi Lu, Arnab Sen, Anders W. Sandvik, Cenke Xu, and Zi Yang Meng, Duality between the deconfined quantum-critical point and the bosonic topological transition, Phys. Rev. X 7, 031051
4. Zhen Bi, Ruixing Zhang, Yi-Zhuang You, Andrea Young, Leon Balents, Chao-Xing Liu, and Cenke Xu, Bilayer Graphene as a Platform for Bosonic Symmetry-Protected Topological States, Phys. Rev. Lett. 118, 126801
5. Yi-Zhuang You, Zhen Bi, Alex Rasmussen, Kevin Slagle, Cenke Xu, Wave Function and Strange Correlator of Short Range Entangled states, Phys. Rev. Lett. 112, 247202

**(d) Synergistic Activities**

Co-PI for the Gordon and Betty Moore Foundation program "Emergent Phenomena in Quantum Systems", in University of California, Santa Barbara

1. Referee for Science, Nature, Nature Physics, Nature Communications, Physical Review Letter, Physical Review X, etc.
2. Reviewer for National Science Foundation, and Department of Energy

## 16 HONORS AND AWARDS IN THIS REPORTING PERIOD

### MRL FACULTY HONORS/AWARDS 2017-18

**Chmelka, Bradley**
Elected Foreign member, Royal Swedish Academy of Engineering, October 2017

**Daly, Samantha**
Robert Caddell Memorial Materials & Manufacturing Award (with graduate student Will LePage and co-advisor John Shaw), The University of Michigan, 2018
Conference Plenary, The British Society for Strain Measurement, 2017

**Fredrickson, Glenn**
Materials Theory Awards of the MRS, November 2017
Seoul National University Chemical and Biological Engineering Distinguished Lectureship, January 2018

**Hawker, Craig**
Named Lectureship - Barré Lectures, University of Montreal, 2017
Named Lectureship - Covestro Lectures, University of Pittsburgh, October 2017
Named Lectureship - Axelta Lecturer, University of Pennsylvania, October 2017
Named Lectureship - Overberger Lecturer, University of Michigan, October 2017
Named Lectureship - MilliporeSigma Lecture, Georgia Institute of Technology, 2017
Named Lectureship - Dauben Lecturer, University of Washington, 2017
Named Lectureship - Aldrich Lecturer | University of Colorado, Boulder, September 2017

**Songi Han**
Alex Schrader, graduate student, Graduate Division Dissertation Fellowship, UC Santa Barbara, 2017

**Jayich, Ania**
Dolev Bluvstein, undergraduate student, Goldwater Award, 2017
Dolev Bluvstein, undergraduate student, Microscopy Society of America Undergraduate Research Scholarship, 2017
Susanne Baumann, postdoctoral scholar, Swiss National Science Foundation Postdoctoral Fellowship, 2017
Simon Meynell, graduate student, NSERC Postgraduate Scholarship, 2018

**Robert McMeeking**
Tiscornia Lecturer, University of Genoa, Italy, November 2017
Penner Distinguished Lecturer, UC San Diego, February 2018

**Tresa Pollock**
TMS Alexander Scott Distinguished Service Award, 2018
Honorary Member, American Institute of Mining, Metallurgical and Petroleum Engineers, 2018
TMS Morris Cohen Award for Outstanding Contributions to the Science and Technology of Materials, 2018
Department of Defense Vannevar Bush Fellow, 2017

**Seshadri, Ram**
Silver Jubilee Award of the Materials Research Society of India, February 2018

**Valentine, Megan**
Menaka Vilhelm, graduate student, AAAS Mass Media Fellow, 2017
Marcela Areyano, graduate student, NSF LSAMP Brides to the Doctorate Fellowship, 2017

**Van der Walle**
Wennie Wang, graduate student, Silver Medal, MRS, 2017

**Wilson, Stephen**
Rebecca Dally, graduate student, APS GMAG Dissertation Award, 2017

## 17. HIGHLIGHTS

Provided separately in the prescribed PowerPoint format.

## 18. STATEMENT OF UNOBLIGATED FUNDS

There are $0 of unobligated funds.

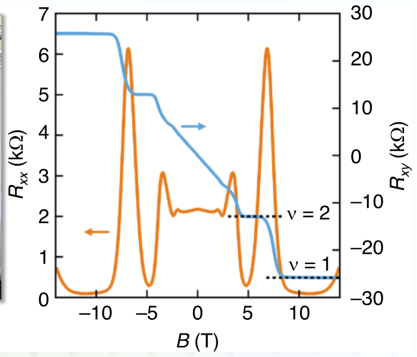
NSF-DMR-1720256
2018 Highlight

## Milli-Kelvin Measurements on $Cd_3As_2$ Films

University of California Santa Barbara

The newly-installed Oxford Triton dilution refrigeration system maintains a 20 mK environment with a 14 T magnetic field enabling the observation of quantum surface states in ultra-thin films.

This milli-Kelvin system acquired with support from the NSF MRI program, is one of the first at a University Shared Facility.




Schumann, Galletti, Kealhofer, Kim, Goyal, Stemmer, Observation of the quantum hall effect in confined films of the three-dimensional dirac semimetal $Cd_3As_2$, *Phys. Rev. Lett.* **120** (2018) 016801.
DOI: 10.1103/PhysRevLett.120.016801

Left panel: Postdoctoral fellow Dr. Luca Galletti loading a sample into the Triton system. Right panel: The quantum Hall effect in a 20-nm-thick epitaxial $Cd_3As_2$ film grown by molecular beam epitaxy. The Hall ($R_{xy}$) and longitudinal ($R_{xx}$) resistances measured at $T$ = 1 K are displayed as a function of magnetic field.

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NSF-DMR-1720256
2018 Highlight

## UCSB MRSEC Maker Activities

University of California Santa Barbara

Teachers (left) and K-12 students (middle and right) engage in soft robotic maker activities led by UCSB MRSEC graduate student volunteers.

In response to the needs of teachers, the UCSB MRSEC has placed a new focus on the development of *maker activities* for K-12 students. These encourage the integration of maker activities into the school curriculum as well as within out-of-school environments (*Maker Faires*), supporting the adoption of Next Generation Science Standards (NGSS).

NSF DMR DIVISION OF MATERIALS RESEARCH
DIRECTORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES

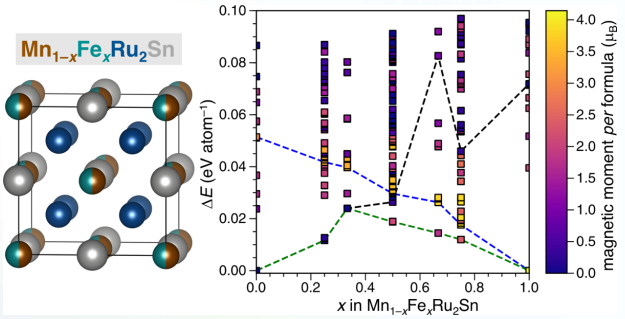
NSF-DMR-1720256
2018 Highlight

## IRG-1: Competing Magnetism in Heusler Compounds

University of California Santa Barbara

**Intellectual Merit:** The alloy $Mn_{0.5}Fe_{0.5}Ru_2Sn$ — formed as a solid-solution of two Heusler compounds — has been shown to exhibit exchange hardening suggestive of two magnetic phases, despite existing as a single chemical phase. A computational study of the chemical and magnetic degrees of freedom in this system have helped to determine the origin of the unusual magnetic behavior.

**Broader Impacts:** The research suggests a simple means of tuning useful magnetic materials.




Crystal structure depiction of the Heusler solid-solution $Mn_{1-x}Fe_xRu_2Sn$ solid-solution (left panel) and the computed evolution of the magnetic behavior, compared with experimental data, which is depicted at the bottom of the plot (right panel).

Decolvenaere, Gordon, Seshadri, Van der Ven, First-principles investigation of competing magnetic interactions in Heusler (Mn,Fe)$Ru_2Sn$ solid solutions, *Phys. Rev. B.* **96** (2017) 165109(1–12). [DOI: 10.1103/PhysRevB.96.165109]

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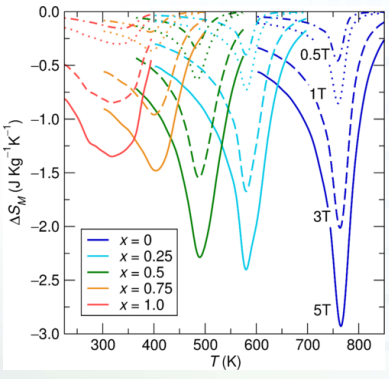
NSF-DMR-1720256
2018 Highlight

## IRG-1: Magnetocaloric Heusler Solid-Solutions

University of California Santa Barbara

**Intellectual Merit:** A study of the magnetic $MnNi_{1+x}Sb$ solid solution between the half-Heusler and Heusler end members reveals magnetocaloric behavior for all samples with a maximum in the refrigerant capacity at $x = 0.75$. The Curie temperature of this system is highly tunable between 350 K and 750 K.

**Broader Impacts:** The properties of the materials make them of interest for refrigeration and for low grade waste heat recovery *via* thermomagnetic power generation.




Magnetic entropy change for various applied maximum fields in the half-Heusler/Heusler $MnNi_{1+x}Sb$ solid-solution.

The temperature tunability, and the increased transition width in the Heusler-rich compositions, are notable.

Levin, Bocarsly, Wyckoff, Pollock, Seshadri, Tuning the magnetocaloric response in half-Heusler/Heusler $MnNi_{1+x}Sb$ solid solutions, *Phys. Rev. Mater.* **1** (2017) 075003(1–8). [DOI: 10.1103/PhysRevMaterials.1.075003]

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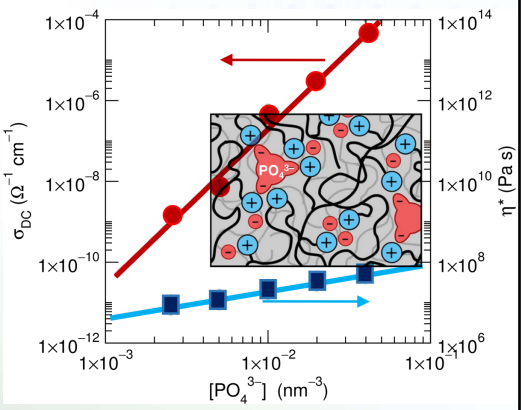
NSF-DMR-1720256
2018 Highlight

## IRG-2: Evolution of Ion Transport and Mechanics

University of California Santa Barbara

**Intellectual merit:** The mechanical properties of an ion-containing polymeric ionic liquid (PIL) can be controllably altered through exchange of monovalent anions (chloride) with trivalent anions (phosphate). This produces significant changes in both the modulus and the ionic conductivity of the PIL for very small degrees of ion substitution as illustrated here (data taken at $T$ = 50 °C).

**Broader Impacts:** The potential to tune the mechanical and conductive responses of PILs through simple ion exchange for multivalent anions presents a new route, and new opportunities for tailoring the macroscopic properties of ion-conducting materials.




Bartels, Sanoja, Evans, Segalman, Helgeson, Decoupling mechanical and conductive dynamics of polymeric ionic liquids via a trivalent anion additive, *Macromolecules* **50** (2015) 8979−8987. DOI: 10.1021/acs.macromol.7b01351

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NSF-DMR-1720256
2018 Highlight

## IRG-2: Controlling Triple-Helix Formation

University of California Santa Barbara

**Intellectual merit:** Poly(methyl methacrylate) (PMMA) forms a stereocomplex that is a unique example of a multistranded synthetic helix. Discrete stereoregular oligomer libraries prepared by combining stereospecific polymerization techniques with automated flash chromatography purification lead to precise building blocks allowing exquisite control of helix formation.

**Broader Impacts:** The understanding that has emerged from this study presents new opportunities for the development of next-generation polymeric materials based on a triple-helix motif.

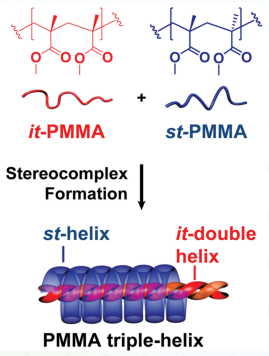


Illustration of stereocomplex formation of a poly(methyl methacrylate) triple-helix. "*st*" and "*it*" refer to distinct polymer arrangements.

Ren, Lawrence, Knight, Abdilla, Bou Zerdan, Levi, Oschmann, Gutekunst, Lee, Li, McGrath, Bates, Qiao, Hawker, Controlled formation and binding selectivity of discrete oligo(methyl methacrylate) stereocomplexes, *J. Am. Chem. Soc.* **140** (2018) 1945−1951. DOI: 10.1021/jacs.7b13095

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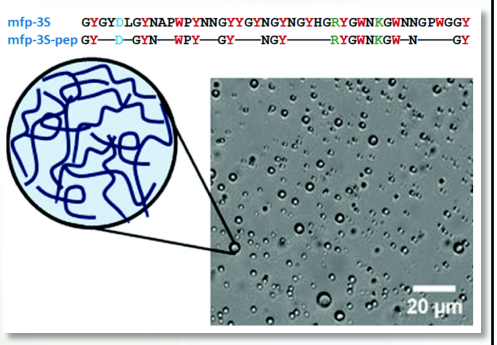
NSF-DMR-1720256
2018 Highlight

## IRG-3: Simple Coacervation of a Mussel-inspired Peptide Improves Wet Adhesion

University of California Santa Barbara

**Intellectual merit:** Upon spontaneous deposition on surfaces underwater and moderate compression, single-component coacervates of adhesive peptide mimics (mfp-3S-pep) display orders of magnitude improvement compared with un-coacervated native (mfp-3S) or synthetic peptides. The increase in the work of adhesion is due to the peptide's intrinsic cohesive properties upon coacervation correlated with dehydration, tight peptide packing and restricted peptide mobility.

**Broader Impacts:** Dense single-component coacervate liquids represent an essential adaptation for the priming stages of mussel adhesive deposition, and provide a previously untapped design principle for synthetic underwater adhesives.




Mfp3-2S-pep is a mimic of the actual mussel-foot protein that helps mussel adhesion (sequences displayed at the top). This mimic undergoes single component coacervation, thereby enhancing adhesion.

Kaminker, Wei, Schrader, Talmon, Valentine, Israelachvili, Waite, Han, Simple peptide coacervates adapted for rapid pressure-sensitive wet adhesion, *Soft Matter* 13 (2017) 9122–9131. DOI: 10.1039/C7SM01915G

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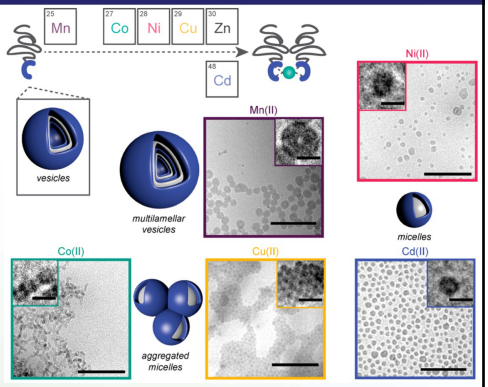
NSF-DMR-1720256
2018 Highlight

## IRG-3: Controlled Amphiphile Self-Assembly *via* Bioinspired Metal Ion Coordination

University of California Santa Barbara

**Intellectual merit:** Peptide-polymer conjugates have been designed and synthesized that exhibit metal coordination-sensitive self-assembly similar to natural siderophores. The assembled morphology of these hybrid amphiphiles is highly sensitive to the strength of metal coordination, as evident by significant morphological shifts observed in cryo-TEM measurements upon exchange of various transition metal ions.

**Broader Impacts:** Metal ion coordination presents a trigger for the hierarchical structuring of soft materials that is distinct from other mechanisms, and can further be used to introduce physical bonding schemes between molecules and assembled interfaces to tailor their mechanical properties.




Scale bars are 200 nm or 20 nm for the insets.

Knight, Larsson, Ren, Zerdan, Seguin, Vrahas, Liu, Ren, Hawker, Controlled amphiphile self-assembly via bioinspired metal ion coordination, *J. Am. Chem. Soc.* **140** (2018) 1409−1414. DOI: 10.1039/C7SM01915G

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