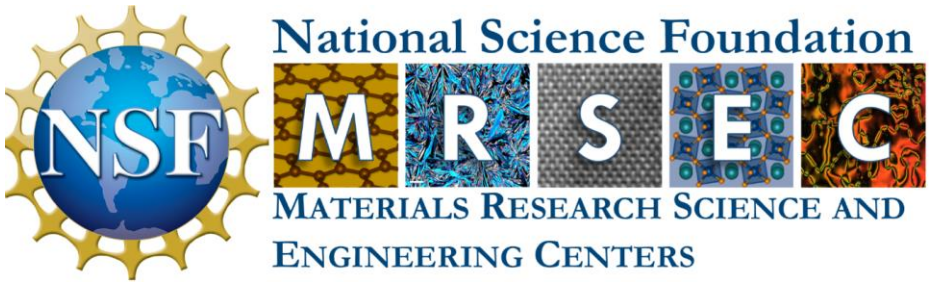
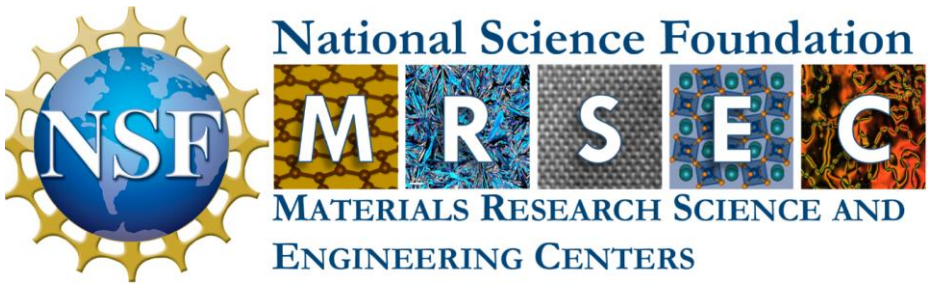
2019 MRSEC Directors Meeting and iSuperSeed2 Workshop

October 3, 2019
Holiday Inn Carlyle
Alexandria, VA

Dan Finotello and Miriam Deutsch
MRSEC Program Directors



A Workshop Reviewing the iSuperSeed2 Accomplishments Sept. 2018 – Sept. 2019



Attendees

UCSB	Ram Seshadri	Cristina Marchetti	
Wisconsin	Paul Voyles		
UIUC	Nadya Mason	Taylor Hughes	Vidya Madhavan
Northwestern	Mark Hersam	Will Dichtel	
Minnesota	Tim Lodge	Rafael Fernandes	Vlad Pribiag
NYU	Marcus Weck		
Cornell	Frank Wise	Eun-Ah Kim	
Brandeis	Seth Fraden	Anique Olivier-Mason	
Chicago	Margaret Gardel	Arvind Murugan	Sidney Nagel
Princeton	Ali Yazdani	Howard Stone	
Ohio State	Chris Hammel	Ezekiel Johnston-Halperin	
Columbia	Jim Hone	Latha Venkataraman	Colin Nuckolls
Penn State	Vin Crespi	Beth Elacqua	
UT Austin	Ed Yu	Eric Anslyn	Tanner Jerome Geibel
Harvard	David Weitz	Jennifer Lewis	Robert Graham
Colorado	Noel Clark	Christine Morrow	
MIT	Geoffrey Beach		
Nebraska	Rebecca Lai		
U of Washington	Daniel Gamelin	David Ginger	
U Penn	Arjun Yodh	Matthew Good	Daniel Hammer
NSF	Dan Finotello		
NSF	Miriam Deutsch		
NSF	Alex Klironomos		
KZN Consulting	Divya Abhat		
KZN Consulting	Ashish Tonse		

DMR MRSEC
2018 iSuperSEED2 Supplements Competition Announcement

Thanks to the remarkable efforts of the Division Director, Linda Sapochak, and the Deputy Division Director, Sean Jones, the Materials Research Science and Engineering Center program of the Division of Materials Research is making available, depending on funds availability, 4-6 iSuperSEED2 Supplements to existing MRSEC awards, 2014 and 2017 Classes. The iSuperSEED2 topics of interest must be part of the current DMR research portfolio, and for this specific call they must be aligned with DMR's participation in the NSF Big Ideas described here:

(a) **The Quantum Leap:** Leading the Next Quantum Revolution: Exploiting quantum mechanics to observe, manipulate, and control the behavior of particles and energy at atomic and subatomic scales, resulting in next-generation technologies for sensing, computing, modeling, and communicating.

https://www.nsf.gov/news/special_reports/big_ideas/quantum.jsp

(b) **Understanding the Rules of Life**: Predicting Phenotype: Elucidating the sets of rules that predict an organism's observable characteristics, its phenotype. Life on our planet is arranged in levels of organization ranging from the molecular scale through to the biosphere. There exists a remarkable amount of complexity in the interactions within and between these levels of organization and across scales of time and space

https://www.nsf.gov/news/special_reports/big_ideas/life.jsp

(c) **Harnessing the Data Revolution:** Engaging NSF's research community in the pursuit of fundamental research in data science and engineering, the development of a cohesive, federated, national-scale approach to research data infrastructure, and the development of a 21st-centurydata-capable workforce.

https://www.nsf.gov/news/special_reports/big_ideas/harnessing.jsp

(d) **The Future of Work at the Human-Technology Frontier:** Understanding how constantly evolving technologies are actively shaping the lives of workers and how people in turn can shape those technologies, especially in the world of work. The future of work at the human-technology frontier will bring together NSF research communities to conduct basic scientific research on the interaction of humans, society, and technology that will help shape the future of work to increase opportunities for workers and productivity for the American economy.

https://www.nsf.gov/news/special_reports/big_ideas/human_tech.jsp

(e) **Growing Convergence Research at NSF:** Framing challenging research questions at inception, and fostering the collaborations needed for successful inquiry. The grand challenges of today -- protecting human health; understanding the food, energy, water nexus; exploring the universe at all scales -- will not be solved by one discipline alone. They require convergence: the merging of

ideas, approaches and technologies from widely diverse fields of knowledge to stimulate innovation and discovery.

https://www.nsf.gov/news/special_reports/big_ideas/convergent.jsp

(f) **NSF INCLUDES (Inclusion across the Nation of Communities of Learners of Underrepresented Discoverers in Engineering and Science):** Enhancing STEM through Diversity and Inclusion: Transforming education and career pathways to help broaden participation in science and engineering. NSF has funded 67 launch pilots to date. The focus of these NSF INCLUDES launch pilots spans a number of broadening participation activities – from STEM engagement and preparatory experiences for students and other community members to educator training to new academic programs that expand access to STEM education.

https://www.nsf.gov/news/special_reports/big_ideas/includes.jsp

Agenda

Thursday October 3, 2019; Holiday Inn Carlyle

7:30 - 8:00 Breakfast

Session 1. Chair: Mark Hersam, Northwestern University – Quantum Leap

8:00 - 8:40	NSF/DMR/MRSEC	Dan Finotello, Miriam Deutsch, Alex Klironomos	
8:40 - 9:00	iSS Presentations	Taylor Hughes, UIUC	QL
9:00 - 9:20		Rafael Fernandes, Minnesota	QL
9:20 - 9:40		Zeke Johnston-Halperin, Ohio State	QL
9:40 - 10:00		Latha Venkataraman, Columbia	QL

10:00 - 10:20 Coffee Break

Session 2. Chair: Frank Wise, Cornell University – Rules of Life

10:20 - 10:40	Cristina Marchetti, UCSB	RoL
10:40 - 11:00	Arvind Murugan, Chicago	RoL
11:00 - 11:20	Howard Stone, Princeton	RoL
11:20 - 11:40	Beth Elacqua, Penn State	RoL
11:40 - 12:00	Matthew Good, U Penn	RoL

12:00 - 1:30 Lunch Working Groups - Reports

Session 3. Chair: Frank Wise, Cornell University – Convergence and Includes

1:40 - 2:00	David Weitz, Harvard	Conv./RoL
2:00 - 2:20	Will Dichtel, Northwestern	Conv.
2:20 - 2:40	Seth Fraden, Brandeis	Includes
2:40 - 3:00	Christine Morrow, Colorado/UCSB	Includes

3:00 - 3:20 Coffee Break

Session 4. Chair: Mark Hersam, Northwestern University – Harnessing Data

3:20 - 3:40	Eun-Ah Kim, Cornell	HD
3:40 - 4:00	David Ginger, Washington	HD
4:00 - 4:20	Eric Anslyn, UT Austin	HD/RoL

NSF Big Idea

Quantum Leap

The Quantum Leap: Leading the Next Quantum Revolution: Exploiting quantum mechanics to observe, manipulate, and control the behavior of particles and energy at atomic and subatomic scales, resulting in next-generation technologies for sensing, computing, modeling, and communicating.

https://www.nsf.gov/news/special_reports/big_ideas/quantum.jsp

NSF MRSEC SuperSeed: Higher-Order Topological Phases of Matter

Investigators: Taylor L. Hughes (PI), Vidya Madhavan, Dale J. Van Harlingen, **UIUC**

We are exploring a new class of topological electronic materials, known as ***Higher-Order Topological Phases (HOTP)***. Unlike conventional topological insulators (TIs), HOTPs are not characterized by gapless surface states. Instead they have stable, gapless modes on "higher-order" surfaces, i.e., places where multiple surfaces intersect at hinges and corners (or similar defects). These localized states are predicted to be useful for quantum information processing with the advantage that they can be precisely designed and placed using standard fabrication techniques. Our goal is to verify their existence, characterize their electronic properties, and determine their potential for quantum information and sensing applications in alignment with the NSF Big Idea Quantum Leap.

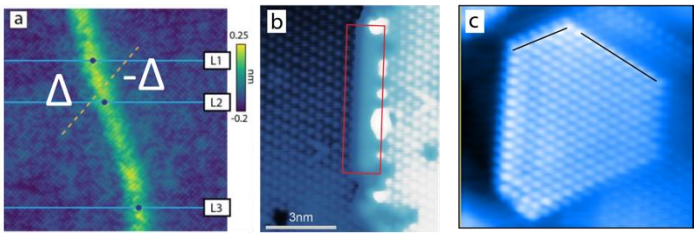


Figure 1. (a) Domain wall defect on surface of superconducting $FeSe_xTe_{1-x}$ *(b) Chiral terrace states on* $Co_3Sn_2S_2$ *surface (c) Hinge-like states on triangular defects on Bi films*

In our experimental work we have focused on three materials that have been predicted to have higher-order or related phenomena. First we have studied the topological superconductor $FeSe_xTe_{1-x}$. This material has a normal metal state that coexists with topological surface states. It is superconducting at around 14K and has been shown to have features of topological superconductivity. The nature of the order parameter is not fully known, and some theory work predicts higher order topological superconductivity. In our work we identified a crystal defect on the surface that traps a channel of helical Majorana modes (see Fig. 1a). The crystal defect generates a pi-phase slip domain wall of the surface superconductivity which acts to trap the Majorana modes. This work shows features that are compatible with higher order topology, and may help to identify the nature of the superconducting order parameter in $FeSe_xTe_{1-x}$. (Article submitted)

The second system we considered is $Co_3Sn_2S_2$ which is a time-reversal breaking Weyl semimetal. All Weyl semimetals effectively arise from strongly coupled layers of 2D Chern (quantum anomalous Hall) insulators that exhibit chiral edge states. We find that surface terrace defects can serve to isolate plateaus of Chern insulators that exist between steps of the terrace. We have found experimental evidence, backed up by our theory, of chiral edge states that exist on these surface step defects (see Fig. 1b). (Article submitted)

Finally, we have been exploring higher order topology in $Bi_{1-x}Sb_x$. Bi has been predicted to be a higher order TI with helical hinge states, and there is some tantalizing experimental evidence for this in bulk Bi crystals. Bi is a semimetal so we have been trying to generate insulating samples of Bi by growing thin films and combining with Sb. We have confirmed the existence of localized modes on triangular defects in Bi films (see Fig. 1c), and furthermore have shown that these signatures disappear once a nominal amount of Sb is added. This indicates that there is a topological transition as a function of Sb content that changes the nature of the defect states (possibly the previously studied band inversion transition). There is controversy in the literature on the (conventional and higher order) topological nature of both Bi and Sb. Our work will help untangle this conflict and determine if either Bi or Sb is a higher order TI.

We have also completed four theory projects on related topics. We have (i) developed the first many-body tool to calculate electric multipole moments in crystals, (ii) predicted new types of 3D higher order topological superconductors, (iii) predicted fractionalized charge on disclination defects in higher order TIs, and (iv) predicted vortex and surface topological phase transitions in s-wave proximitized higher order TIs. (One article published, three others submitted.)

In summary we have submitted six articles in the first year and made multiple exciting experimental discoveries, several of which will clearly impact the topological material community and beyond.

iSuperSeed2 Project: **Bridging the 2D and 3D Worlds with Transition Metal Dichalcogenides**
(PIs: Turan Birol, Fiona Burnell, Rafael Fernandes, Vlad Pribiag, and Ke Wang, **U of Minnesota**).

Our aim is to explore the unique properties of transition metal dichalcogenides between the bulk and monolayer limits. The motivation is to combine properties typically observed in the 3D limit, such as superconductivity and charge-density waves, with features that are typical of the 2D limit, such as strong spin-orbit coupling and topological properties. The overarching goal is to search for novel electronic quantum states that take advantage of features typical of these two regimes, elevating these fascinating materials to the forefront of the next quantum revolution in the Quantum Leap. Two systems were investigated in joint theoretical-experimental efforts: $NbSe_2$ and WTe_2. Both display superconductivity in monolayer form. In the case of $NbSe_2$, the Cooper pairs form in the presence of strong Ising spin-orbit coupling. In the case of WTe_2, a superconducting state emerges after enough carriers are added to a quantum spin-hall insulating phase.

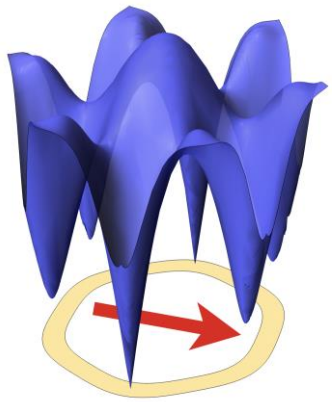


Figure 1. The predicted crystalline nodal topological superconducting gap along the Γ pocket of $NbSe_2$. Two nodes are present along the direction perpendicular to that of the applied magnetic field **B**.

For the former, we developed the first microscopic theory of superconductivity in monolayer $NbSe_2$, and the prediction of a novel crystalline nodal topological superconducting phase, which is very sensitive to the direction of an applied in-plane magnetic field. In particular, at large enough fields and for zero Rashba spin-orbit coupling (SOC), the superconducting state has twelve nodes protected by a time-reversal-like symmetry of the system. A finite Rashba SOC generally lifts these nodes, except when the field is applied along the Γ-K direction. In this case, the four nodes located perpendicular to the field are protected by a mirror symmetry (Fig. 1). If the Cooper pairs have zero momentum, the nodes are shifted in a staggered fashion away from the Fermi level, giving rise to Bogolyubov Fermi surfaces inside the superconducting state. If the Cooper pairs acquire a non-zero momentum, the nodes move to the Fermi level.

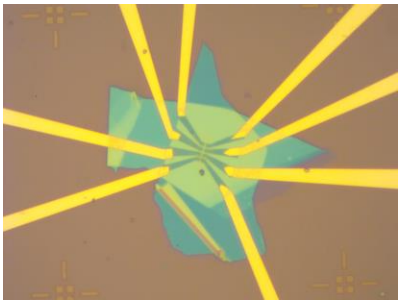


Figure 2. Optical imaging of a high quality trilayer $NbSe_2$ device post-fabrication.

Motivated by these theoretical results, which predict a strong anisotropy of the superconducting properties of monolayer $NbSe_2$, (and possibly odd-layer $NbSe_2$), transport measurements were performed in very clean fully-hBN-encapsulated $NbSe_2$ samples in the few-layer limit (see Fig. 2 for a trilayer device). A remarkable two-fold anisotropy of the magneto-resistance was observed as function of the in-plane direction of the magnetic field. Such an anisotropy only appears between the temperatures corresponding to the onset T_c and the offset T_c, displaying a broad maximum as function of the field magnitude.

For WTe_2, first-principle calculations were performed to elucidate the evolution of the band structure as the number of layers and the carrier concentration are changed. The motivation is to shed light on the previously observed transition from a quantum spin-Hall insulating phase to a superconducting phase induced by gating in monolayer WTe_2. The possible transition to a type-II Weyl semi-metal as the number of layers increases towards the bulk limit is another major motivation. Edge states were determined for distinct geometries and numbers of layers. The Fermi surface that emerges as negative carriers are introduced into the system was also obtained. It was found that the orbital content of the Fermi surface displays a strong anisotropy as the angle across the Fermi surface varies. In particular, certain portions of the Fermi surface have a strong W d-orbital-character, whereas others display dominant Te p-orbital-character. Such behavior is expected to be manifested as a strong anisotropy in the gap function in the superconducting state.

Materials for Hybrid Quantum Interfaces

Flatté, Gauthier, Gupta, Johnston-Halperin, Kawakami, **Ohio State University**

Goals and Research Activity: The goal of our iSuperSeed program is to lay the foundations for a research program exploring transduction between multiple quantum coherent degrees-of-freedom across hybrid quantum interfaces. Specifically, our vision encompasses the development of novel spin-qubits through the encapsulation of point defects in 2D materials and adatoms of selected atomic species within mechanically assembled 2D heterostructures. These heterostructures in turn can be readily integrated with low-loss organic-based magnetic structures to enable hybrid qubits based on coherent spin-magnon-spin coupling. This effort requires close coupling between materials development and the illumination of fundamental physical processes. During the period of this seed award we have achieved a number of technical and scientific milestones, which can be grouped into the following three thrust areas.

Encapsulation: We have developed a variety of UHV-compatible h-BN transfer processes, including UHV exfoliation transfer from commercial crystals and CVD-grown films onto multiple substrates: i) Eu deposited on MgO surfaces: we performed low temperature PL microscopy, where we observe characteristic light emission from the Eu^{2+} state. ii) UHV-cleaved GaAs: this provided a pristine surface to realize the cleanest possible interface w/ hBN. In addition, we have succeeded in direct UHV growth of hBN on Cu(100) and dropcasting of submicron hBN flake powder suspended in UHV-friendly solvents onto HOPG and Au(111) surfaces. Finally, we developed air-free approaches to encapsulation of potential molecular qubits. We have successfully encapsulated Cy3 and Cy5 fluorophores to validate this approach.

Coherent single-photon spectroscopy: We have developed a correlated-emission microscope, including integration with PL microscopy (described above) to detect optical emission from point defects in h-BN or atoms encapsulated in h-BN. The single-photon detectors are silicon single-photon avalanche photodiodes with high quantum efficiency in the visible and near infrared part of the spectrum with a sub-nanosecond jitter. Fluorescent light from the optical emitter is coupled into a multi-mode fiber, split with a 50:50 multimode coupler, and directed to the single-photon detector. A low-jitter time-to-digital converter time-tags the events from each detector and off-loads the data to a personal computer. The system has been validated with weak coherent light from a laser. Measurements of encapsulated samples are ongoing.

Modeling of candidate atomic species: To identify atoms that will serve as qubits when encapsulated by h-BN, we use the following criterion: 1) neutral or singly ionized atoms; 2) ground states with orbital + electron spin J=1/2, J=1/2 and 3/2, or J=0 and 1; 3) low nuclear spin (preferably $I \leq 1$); and 4) strongly allowed optical transitions that fall within the bandgap of h-BN. Our current candidate atoms are: A) neutral thallium (J=1/2 and J=3/2, I=1/2) with a fine-structure splitting corresponding to a transition wavelength of 1.28 μm in the short-wave telecommunication band for direct spin pumping and an allowed optical transition at 377 nm for indirect spin pumping; B) singly-ionized ytterbium-171 (J=1/2, I=1/2) with a hyperfine splitting of 12.6 GHz for direct spin pumping and a strongly allowed optical transition at 370 nm for indirect spin pumping; and C) neutral rubidium-87 (J=1/2, I=3/2) with a hyperfine splitting of 6.8 GHz for direct spin pumping and a strongly allowed optical transition at 780 nm for indirect spin pumping. To investigate these systems theoretically, we are using analytic methods for obtaining approximate energy levels and configuration assignments, followed by density-functional-theory simulations for highly accurate predictions.

Outcomes of iSuperSeed Funding: The results described above have provided critical foundational data for the development of a comprehensive research program. Efforts are ongoing, but to date the molecular encapsulation efforts have resulted in the successful competition for an NSF TAQS award for 3 of the iSuperSeed PIs (Flatté, Gupta, Johnston-Halperin) along with a new collaborator (Prof. Danna Freedman, Chemistry, Northwestern). We anticipate similar success for the atomic encapsulation strategies. In addition, our seed program has supported the training of 5 PhD students (including two women) in an interdisciplinary and collaborative environment. One of those students has graduated and is currently a postdoc in the Fuchs group at Cornell.

Columbia MRSEC iSuperSeed2: Synthetic Networks in Quantum Materials

PI: Dmitri N. Basov db3056@coulumbia.edu; co-PI: Latha Venkataraman lv2117@columbia.edu

Senior participants: Ana Asenjo Garcia *(Columbia Physics)*, Michal Lipson *(Columbia Electrical Engineering)*, Xavier Roy *(Columbia Chemistry)*, James Schuck *(Columbia Mechanical Engineering)*

The primary goals of this iSuperSeed2 were to design, create and characterize: *i)* light emitting and magnetic molecular components; *ii)* new architectures of layered quantum materials displaying rich moiré patterns; and *iii)* entirely novel quantum networks based on the combination of *i)* and *ii)* that are addressable and tunable. In order to achieve these goals, the team combines molecular synthesis with two-dimensional materials, and utilizes advanced scanning probe techniques to investigate local electronic structure, optical and electronic phenomena across tunable lengths scales.

During the past year, the team has made a number of advances towards these goals with both fundamental intellectual merit and broader impacts. These fall in two broad categories, both focused on developing techniques to observe light emission at the nanoscale: the first aims to image stacked layered materials in the near field and infrared, and the second aims to observe light emission from molecular components. We have made major progress towards both goals during this past year as detailed below.

We fabricated monolayer-on-monolayer hexagonal boron nitride (hBN) structures with a large range of twist angles as a model system for achieving controllable moiré patterns. We calculated the band structure of the bi-layer structures in a continuum model, and found that for small twist angles, additional flat bands are seen within the gap, leading to sharp spectral features in the density of states that should lead to sharp resonances in optical spectra below the bulk bandgap. We imaged these layered stacks in the near field and found rich moiré patterns with varied periodicity due to strain and atomic reconstruction in hBN membranes. We are working towards improving our spectroscopic capabilities to observe the predicted resonances. The symmetry of stacked bilayer hBN depends on the relative angle of the two layers. Theoretically, when they are rotated by 60 degrees, there is no inversion symmetry, which implies that one should be able to see second-harmonic generation (SHG). We are also working on exploring SHG using atomic force microscopy with nano-IR characterization and also developing the theoretical framework to understand the SHG signatures in twisted hBN.

We have incorporated a photodetector within an existing scanning tunneling microscope and measured electroluminescence from nanoscale tunnel junctions and single-molecule devices. Our preliminary findings are that gold tunnel-junctions emit light with an efficiency that is roughly 1 photon/10^5 electrons. We have in addition measured the spectral dependence of this electroluminescence and found that although most of the light is emitted at an energy lower the applied bias voltage, we do see significant emission above this energy cut-off. This result can only be explained by a two-electron process. We are working towards measuring the emission spectra across single-molecule junctions

The broader impacts of our work during the past year include the implementation of novel nano-imaging and nano-spectroscopy methods, including non-linear nano-spectroscopy that are broadly applicable in physics, chemistry, engineering and materials science. Our scientific accomplishments have been spearheaded by graduate students who are being trained in interdisciplinary research. This research program has integrated a junior faculty member, Professor Ana Asenjo Garcia, who has recently joined the Physics Department into the MRSEC effort. Finally, we are making great progress towards producing high-quality vdW materials with unique optical properties to create a foundation for broader applications of this class of materials in new electronic, photonic, and energy management technologies needed to address the growing societal demands for rapid and energy-efficient information processing and transduction.

NSF Big Idea

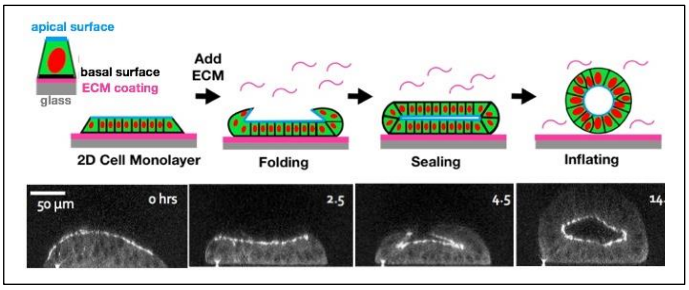
Rules of Life

Understanding the Rules of Life: Predicting Phenotype: Elucidating the sets of rules that predict an organism's observable characteristics, its phenotype. Life on our planet is arranged in levels of organization ranging from the molecular scale through to the biosphere. There exists a remarkable amount of complexity in the interactions within and between these levels of organization and across scales of time and space

https://www.nsf.gov/news/special_reports/big_ideas/life.jsp

UC Santa Barbara Materials Research Laboratory – DMR-1720256
iSuperSeed: *Shape from Activity-Driven Folding: a path to materials morphogenesis*
M. Cristina Marchetti, Zvonimir Dogic, Mark Bowick, Sebastian Streichan

Overview: The challenge addressed by this iSuperSeed is understanding how the shape of organs and organisms emerges from the spontaneous organization of *active* processes at the molecular scale, and applying this understanding to the design of self-shaping materials. The specific research plan is based on the observation that biological structures (organs and organisms) are often achieved by first assembling cells into two-dimensional (2D) tissue layers that then attain the desired form of 3D organs through targeted and repetitive active folding processes. Our goal is to quantify how given 3D folds are determined by specific spatial and temporal distributions of mechanical forces generated in 2D cell sheets by activity at the molecular level.



Research Progress: During the first year of funding we have focused on understanding the mechanisms through which 2D flat single sheets of human stem cells (hSC) undergo large-scale controlled topological changes to fold and close to form *lumina* – 3D hollow spherical or tubular structures as in an artery or the gut. *Lumen* formation is directly relevant to the development of *in vitro* organoids. It is driven by active stresses set up by the correlated action of biomolecules such as myosin motors, and the interaction with the environment provided by the extracellular matrix (ECM). Progress made so far includes: 1) the identification of conditions for the growth and live imaging of hSC; 2) the development of assays to control the folding of 2D hSC sheets and the imaging of the folding process and of the resulting 3D structures; and 3) physical modeling of the onset of the folding process. 1) Postdoctoral fellow Eyal Karzbrun has successfully identified live imaging conditions consistent with the reported 18 hours doubling time of the hSC lines and has demonstrated the feasibility of the use of confocal and light sheet microscopes for rapid imaging of fluorescent labeled samples at subcellular resolution. 2) We developed a procedure to control topological changes from 2D flat to closed 3D geometry. To achieve this, we seed a tissue of cells on a gel rich in ECM components and incubate in stem cell media surrounding the tissue for 24 hours. We then supply a dilute amount of the same ECM polymers to the medium, as shown in the cartoon. This triggers the folding transition. The initially flat tissue folds to generate a single large *lumen* (see still images). Fluorescent myosin markers, revealed that the ECM polymers added to the medium mediate a local enrichment of myosin at the tissue perimeter, strengthening the actomyosin cable that surrounds the tissue like a rubber band and drives the closure of the folded tissue, much like the purse string in wound healing. Once closed, the lumen inflates significantly. Using automated image analysis, we measured the length of the actin cable perimeter over time, and identified two regimes: the colony perimeter remains nearly constant over the first 8 hours, then rapidly decrease until tissue folding is completed. Using patterning of the substrate, we have then examined the folding of 2D tissue patches of specific shape (circular, square, triangular) to assess the effect of 2D shape and curvature on the resulting 3D structure. 3) To quantify the relative role of various active processes at the cellular scale in controlling the initial folding instability, postdoc Benjamin Loewe and students Francesco Serafin and Suraj Shankar have developed an effective 2D model of the tissue as an active elastic continuum, incorporating the important anisotropy between apical (top) and basal (bottom) tissue surfaces. The folding instability is controlled by the interplay of contractile forces (from apical myosin) and extensile ones (due to growth and directed cell motility at the tissue edge), and it is tuned in the model by the tension Λ describing the actomyosin cable. Folding is signaled by a change in the sign of the curvature of the apical surface and by ``elastic dewetting'' at the sheet edges. Extensile forces are essential for the onset of folding, and the relative strength of growth and edge motility determines whether the sequence in which change in surface curvature and dewetting will occur upon increasing Λ. This prediction provides a way of testing which of these forces dominates in a given experiment.

UChicago MRSEC iSuperSeed2: **Harnessing training and memory to evolve material functionality**
(**UChicago**: A. Dinner, M. Gardel, A. Murugan, S. Nagel, S. Palmer; **NWU**: M. Driscoll)

Evolution as a tool for materials design and illuminating the rules of life: Materials age and deteriorate over time. However, the memory retained of how a material was previously manipulated can provide a training protocol for creating desired behaviors not found otherwise. We exploit this behavior into a tool to create novel desired functionality in materials. These ideas have their roots both in material science and in biological evolution in which systems adapt by feeding back memories of its previous environment to determine future evolution. The ruggedness of the *genotype-to-phenotype map* dictates if training can be completely greedy or whether it needs to allow for deleterious changes in hope of subsequent larger gains. While many biophysical systems have features with no direct benefit (but reflect their evolutionary development), others, such as proteins and neural networks evolved in changing environments, are adaptable and can switch between functions in a way that designed systems rarely can. Our goal is to understand the scope, limits and benefits of similar training paradigms for materials.

Training as a new Materials Design Principle: Murugan and Nagel have shown how functions can be designed into materials by changing the geometry of structural elements. They explored the equivalent of *letting the material itself decide how to fold* by active training so that the system retains an imprint of advantageous motions during its evolution. Nagel and Murugan's groups have developed techniques in which aging is *directed* so that the bonds that need to be weakened do so naturally. Starting with a material that can plastically deform different tasks can be learned. During compression, bonds or folds under the greatest stress deform fastest. In one example, material transformed from a normal material with positive Poisson's ratio, to one that is highly auxetic with a Poisson's ratio less than $\nu = -0.4$ to evolve an auxetic material (1, 2). In another, an origami sheet was trained to fold in a specific controlled manner (3) , providing insight into evolution of protein structure-function.

Training Dynamics: A learning rule only works in a specific regime of learning rates, given the structure of the input fluctuations. Plasticity that is too fast or too slow cannot successfully learn new behaviors. Palmer and Murugan have developed a framework to study the requirements for learnability and optimal prediction in the context of neuroscience. They have developed general results about training materials to generalize the lessons learned from specific materials systems by incorporating constraints set by the physics of our materials into the optimal learning rules (4). They have explored how to train a mechanical network so that manipulation at one point creates a desired motion at a distant site (5).

Self-training in Active Materials: Dinner, Gardel and Murugan have exploited the response of active materials to their environment in order to train the material itself in a directed manner. Gardel has shown properties of actomyosin assemblies that are suited to our training paradigm (6). Such a rich response allows for more complex training of the bulk in a way not possible in passive materials. Murugan has identified conditions under which such non-equilibrium molecular systems can encode multiple memories. They identify rules that reinforce particular transport patterns.

Adaptability from switching environments: Biology shows numerous examples of highly adaptable materials that can switch between different functions as needed. Direct design has a hard task to identify such small multi-functional slivers of design space. Our training framework mimics the biological evolutionary strategy of changing environments. Dinner, Nagel, and Driscoll have trained two- and three-dimensional materials to switch between distinct allosteric motions with only small modification. They are studying the materials' performance as they vary the (in)compatibility of the motions for which they are being trained.

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Harnessing the Rules of Life to Enable Bio-Inspired Soft Materials (Princeton: Nov. 2018 – present)
PIs: H. Stone (MAE), S. Datta (CBE), A. Košmrlj (MAE), C. Brangwynne (CBE), B. Bassler (MOL)

Our *iSuperSeed2* bridges materials science and biology to answer the question—*how do polymers drive biological function?*—at two scales of biological organization: the intra- and extra-cellular levels. The **Intellectual Merit** is that our work provides insight into the roles of polymers in dictating intra-cellular (e.g. gene regulation) and extra-cellular (e.g. tissue shape, biofilm assembly, morphogenesis) functions. In addition to generating publications, we have engaged in **Broader Impacts** by mentoring young scientists, including undergraduates from underrepresented groups, who are also coauthors on some of our papers. Moreover, our collaborative effort has paved the way for a new IRG in the MRSEC re-application, with an expanded team of PIs focused on harnessing the *Rules of Life* for materials design. Our key results are:

(I) Intracellular phase separation: We developed tools to probe intracellular phase separation (Fig. 1a), which is thought to be driven by passive thermodynamic forces, but prior to our work, tools were lacking to study such multicomponent mixtures. We developed a new approach for constructing phase diagrams by convexification of the free energy function[1]. We discovered that the topology of phase-separated mixtures can be described with graphs (Fig. 1b), which enabled us to generate all topologically distinct morphologies. In parallel, we experimentally characterized dynamics in phase-separated condensates.[2] These advances help to understand how cells control gene expression, polymer interactions to achieve target structures, and our results yield guidelines for designing novel multicomponent phase-separated materials on demand.

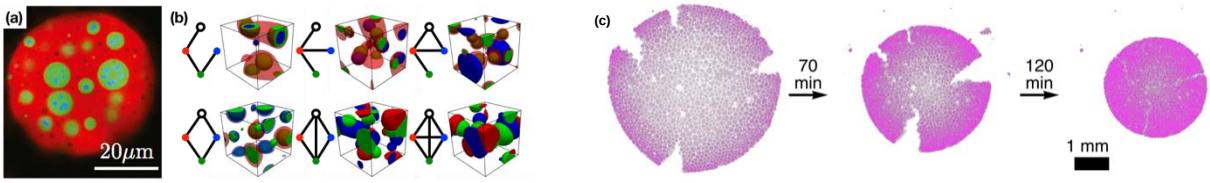

Figure 1. (a) Hierarchical phase separated droplets inside the cell nucleus. (b) Topologically distinct morphologies of four separated phases mixtures with their corresponding graphs. (c) Micrographs showing packing of gel particles (small circles) spontaneously healing cracks upon shrinkage of particles in the center of the packing.[3]

(II) Shape changes of tissue-like assemblies: How cell volume changes in tissues influence macroscopic tissue shape is unknown. To explore this mystery, we developed assemblies of hydrogel particles as models of biological tissues, with tailored drying profiles to control osmotic shrinkage. We discovered[3] that differential shrinkage of particles drives large-scale deformations—even enabling "self-healing" of cracks (Fig. 1c). Our experiments and companion discrete-element simulations establish principles for programming this behavior,[4] demonstrating how tissues can regulate their shapes and potentially self-heal. These findings suggest routes for new functional polymeric materials that can self-heal.

(III) Mechanical instability and interfacial energy drive biofilm morphogenesis: Although structural and regulatory components required for bacterial biofilm formation are known, how they promote biofilm morphology is not understood. Using *V. cholerae*, we combined mechanical measurements, theory, simulations, image analyses, and mutageneses to show that mechanical instabilities, including wrinkling and delamination, underlie morphogenesis of growing biofilms.[5,6] We identified interfacial energy as a driving force that dictates generation of new, and annihilation of existing, interfaces. The principles discovered in biofilms, should be generally applicable to morphogenesis in tissues in higher organisms. We developed the ability to track bacteria within 3D gel matrices. We used this tool to discover a new mode of cellular transport,[7,8] enabling future studies of active matter in confinement.

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[2] N.O. Taylor, M.-T. Wei, H.A. Stone and C.P. Brangwynne *Biophysical Journal*, in press (2019)
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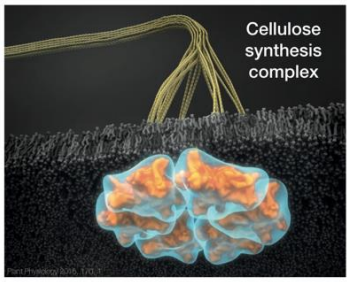
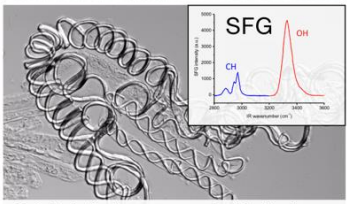
Biologically-Produced Crystalline Nanofibers

Seong Kim, Elizabeth Elacqua, Daniel Cosgrove, Ying Gu, Jeff Catchmark, Lasse Jensen, Zoubeida Ounaies, Venkat Gopalan; Pennsylvania State University

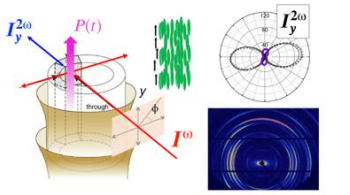
The iSuperSEED aims to deploy Nature's sophisticated synthesis and assembly tactics to produce novel symmetry-enabled functional materials which could not be obtained through purely artificial synthetic approaches: controlling genotype and extracellular stimuli to produce new phenotypes of materials. The lessons learned in controlling nano/meso-scale order then provide new perspectives on mechanisms of supramolecular organization. Converging this NSF/DMR goal in the *Rules of Life* with the expertise of the DOE/EFRC *Center for Lignocellulose Structure and Formation* on cellulose synthesis, the team aims to achieve polar order in crystals built from non-centrosymmetric biopolymers and interrogate unique material properties that originate therefrom, taking advantage of non-equilibrium biological processes to achieve thermodynamically disfavored polar alignments of nanocrystalline domains over macroscopic scales, following three strategies:





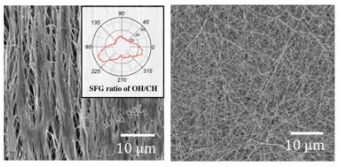
Helicity indicates macroscale chirality, hence non-centrosymmetry

First, to control the movement of cellulose synthesis units to induce polar deposition of microfibrils in biological systems. The team has discovered that cellulose synthesis complexes in induced xylem cells move unidirectionally, not bidirectionally, thus producing polar order in cellulose microfibrils. We have also demonstrated how shear flow at an air/liquid interface induces unidirectional motility in bacteria and thus aligned bacterial cellulose microfibrils.

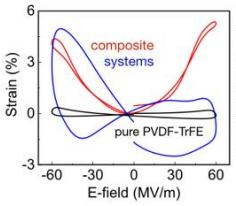


Optical and X-ray evidence of polar order in tubeworm chitin

Second, to identify and exploit natural organisms that already produce polar microfibrils. The team has proven that cellulose microfibrils in the coiled tracheary element of celery are deposited with unidirectional polar order. Investigations on β-chitin, another non-centrosymmetric biopolymer, have confirmed that β-chitin crystalline domains in the tubeworm *Lamellibrachia Satsuma* have uniaxial polar directionality. These discoveries were enabled by expertise in non-linear optical spectroscopy of biological materials that has been established jointly by multiple members of the team. We are currently quantifying the nanoscale electromechanical coupling of these polar-ordered cellulose and β-chitin materials.



Aligned bacteria cellulose grown under shear shows SFG



Composite actuators that combine tubeworm chitin with PVDF-TrFE copolymer show large strain at low field.

Third, to chemically and structurally modify cellulose and β-chitin post-synthesis to enhance material response. Cellulose crystals can be swollen with ammonia and amine solvents; the team is testing if cellulose chains in the solvent-swollen state could be rotated by external electric or magnetic fields. We are also seeking synergistic enhancements in electromechanical coupling when cellulose or β-chitin is fabricated into a composite with electroactive polymers, discover-ing that composites of biopolymers with poly(vinylidene-trifluoroethylene) copolymer can generate extraordinarily large strain responses at relatively low electric fields compared to purely synthetic polymer systems, thus opening new opportunities for lightweight and ultra-strong organic/organic composite actuators.

iSuperseed2 **U Penn**: **Membraneless Organelles with Designed Function from Engineered Assemblies of Intrinsically Disordered Proteins**. Co-Leaders: Matthew Good (CDB) & Elizabeth Rhoades (Chemistry). Dan Hammer (Bioengineering, U. Pennsylvania) & Jeetain Mittal (CBE, Lehigh U.)

A major open question concerning living matter is how cells achieve mesoscale organization of subcellular compartments from the interaction of nanoscale components. Compartmentalization is fundamental strategy to enhance the rate and fidelity of biochemical reactions. In addition to membrane-bound compartments, cells are composed of micron length scale membraneless organelles that display liquid-like properties and are assembled via condensation of proteins and RNA. To date, a grand challenge in understanding the rules of life is to predict the de novo assembly of biomolecular condensates from intrinsically disordered polypeptide (IDP) sequences. A second major challenge is to probe the function of these multi-component condensates in situ. Our approach, which leverages synthetic organelle materials built from genetically encoded components, promises paradigms to decode and extend the functions of protein-based compartments in living and synthetic cell systems.

Expertise: **Rhoades:** single-molecule studies of disordered proteins; **Good:** scaffold proteins; synthetic cell biology; **Hammer**: biomaterials, protein engineering; **Mittal**: coarse-grain modeling of IDP condensation.

Project 1 – Optically Control Protein Assembly and Disassembly
Above a critical concentration, disordered proteins will undergo liquid-liquid phase separation (LLPS). We have developed a unique platform for the self-assembly and phase separation of protein-based organelles from a single IDP domain, though inducible modulation of its critical concentration. Using the disordered RGG domain of the protein Laf-1, we demonstrated that real-time enzymatic alteration of RGG valency enables controllable phase separation (*Schuster … **Good, Hammer**, Nature Communications 2018*). To increase the versatility and kinetic responsiveness of these materials, we have generated two new RGG tools that undergo inducible LLPS to form membraneless organelles using short pulses of light. One approach is based on the photocleavable protein domain, PhoCl. A second is based on light-induced dimerization of RGG domains, which lowers the critical concentration to cross the phase transition boundary.

Project 2 – Develop Orthogonal Biomolecular Condensates Using Simulations and Protein Engineering
A fundamental question is how self-assembly and LLPS is encoded into the primary amino acid sequence of a disordered protein. Using coarse-grain modeling and experimentation we have defined the sequence determinants of protein RGG phase separation (*Dignon, Schuster… **Hammer, Good, Mittal**, Under Revision, PNAS*). Additionally, we have screened for IDP sequences that are orthogonal to RGG - they self-assemble into distinct condensates that do not fuse. Using computational screening, **Mittal** identified a number of mutant RGG sequences as well as distinct IDP sequences that do no co-mix with wildtype RGG. In a complementary approach we have identified orthogonal IDP sequences though co-expression in living cells. **Rhoades** and **Good** have begun purifying candidate IDPs and characterizing their behavior in vitro. Altogether, these results provide insights on the physicochemical principles that control the fidelity of membraneless organelle assembly. From an engineering perspective, we can now express multiple distinct synthetic organelles within cells. Additionally, to regulate the growth and fusion of these organelles, as a proof-of-concept **Hammer** has constructed synthetic surfactant proteins.

Project 3 - Encode programmable membraneless organelles in living cells and cell-like materials
Good and **Hammer** have demonstrated stable formation of synthetic membraneless organelles in 3 mammalian cells lines and in a model single-cell yeast through expression of genetically-encoded RGG sequence variants. These organelles are localized to the cytosol and appear orthogonal to the biology of the cell – they are not cleared by lysosomes or the vacuole and have minimal effect on cell growth. In year 2 of the project, we plan to test expression of these materials in stem progenitor cells and embryonic model systems. Additionally, **Hammer** and **Good** have encapsulated induced the LLPS of RGG materials inside synthetic cell-like compartments.

Outlook: Liquid-liquid phase separation represents a unique paradigm for organizing, concentrating and restructuring constitutive components of biological systems. By developing new tools to engineer and manipulate the properties of membraneless organelles, our studies will provide generalizable insights into the rules of their assembly and how these assemblies direct cell biological functions. This represents an important first step toward the predictive control of function using programmable assembly of organelles that can be genetically encoded and that respond logically to changing environmental conditions.

NSF Big Idea

Convergence

Growing Convergence Research at NSF: Framing challenging research questions at inception, and fostering the collaborations needed for successful inquiry. The grand challenges of today -- protecting human health; understanding the food, energy, water nexus; exploring the universe at all scales -- will not be solved by one discipline alone. They require convergence: the merging of ideas, approaches and technologies from widely diverse fields of knowledge to stimulate innovation and discovery.

https://www.nsf.gov/news/special_reports/big_ideas/convergent.jsp

Materials design principles for cell-based products

Harvard Superseed progress report
MRSEC Directors' Meeting, October 2019

Therapeutic materials are rapidly evolving, moving from small molecules, to large biologics and now to cells. Therapeutic use of cells relies on the specific function of cells themselves, as well as their ability to act as a 'factory' that produces important signaling molecules. The success of this therapy demands encapsulation the cells in materials that both protect them from the natural immune system of the body and enable free flow of nutrients and products from the cells to the surrounding medium. The goal of this project is to draw on different disciplines in the Center and apply "convergence" research to understand the design "rules of the biomaterials" that will enable cell therapy.

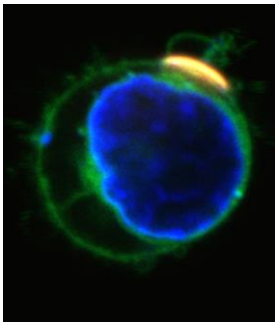


Fig. 1 Backpack (yellow) on macrophage to release cytokines to retain cell phenotype

The focus of much of the work done to date has been on protecting cells and ensuring that the cells are correctly stimulated to enable continued production of signaling molecules. **Mitragotri** is developing disk-shaped particles that release regulatory cytokines (interferon-γ) to ensure that macrophages maintain their immunostimulatory phenotype and interact with the immune system. The challenge is to ensure that these particles remain attached to the surface of the macrophage, and are not internalized by the cells, so their stimulation activity continues over a prolonged time. **Mitragotri** has discovered that controlling the shape of the particles is essential to ensuring their effectiveness, with disc-shaped particles providing the optimum behavior (**Fig. 1**). The macrophages naturally invade tumors and, when stimulated by the 'backpack' polymer discs, can significantly reduce the tumor burden, leading to marked improvement of survival in mouse models for breast and lung cancer. He is continuing to modify both the material structure and shape of the backpacks for further improvement of functionality.

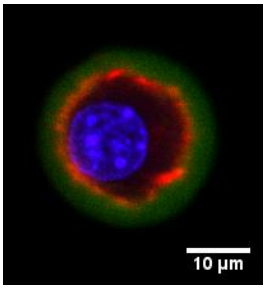


Fig. 2: Stem cell in alginate microparticle (green shell)

Mooney worked with **Weitz** to develop methods to encapsulate stem cells in alginate microparticles to increase their secretion of stimulatory signaling molecules such as inflammation-suppressing paracrine factors. **Mooney** has determined that control of both the stiffness and the relaxation time of the elastic alginate network can modify gene expression to optimize secretion. He has developed modified alginate that forms gels with the optimum behavior. He worked with **Weitz** to use drop-based microfluidics to create microparticles comprised of these alginate gels to encapsulate stem cells. These microparticles protect the stem cells from the immune system while still enabling nutrients to enter the microcapsules and the signaling molecules to exit them. The encapsulated stem cells exhibit improved secretion and much longer retention in mouse models. These encapsulated stem cells are particularly effective for bone marrow applications where protection from the immune system is essential. **Mooney** has extended this work to develop materials to assist in T-cell expansion and a Center graduate student has already spun out this technology into a startup, Immulus, for therapeutic applications.

iSuperSeed2: Molecularly Precise Membranes for Efficient Chemical Separations

William Dichtel (lead)**, Northwestern (**NU) Chemistry; **Omar Farha**, NU Chemical and Biological Engineering; **Nathan Gianneschi**, NU Chemistry and Materials Science and Engineering; **Benito Mariñas**, University of Illinois at Urbana-Champaign Environmental Engineering; **Monica Olvera de la Cruz**, NU Materials Science and Engineering

Our objective is to understand how to assemble molecular building blocks of framework materials (metal-organic frameworks, MOFs; covalent organic frameworks, COFs) into large-area thin films compatible with membrane fabrication processes. The precise and designed porosity of these structures are thought to be ideally suited for energy-efficient chemical separations, yet control of their nucleation and growth processes is needed to create highly crystalline, large-area thin films.

Using a recently developed interfacial polymerization process, three COF films were incorporated as active layers into separate thin-film composite (TFC) membranes and tested for rejection of an organic pollutant surrogate and salt from water. The synthesized membranes consist of a polyacrylonitrile (PAN) membrane supporting COFs with identical hexagonal topologies and pendant groups of progressively increasing size in the pores (–H, $–CH_3$, $–CH_2CH_3$), such that the effective pore size decreases across the series. Once films of comparable thickness were synthesized and transferred to the PAN support, the resulting TFC membranes showed increased rejection of an organic dye (Rhodamine-WT) and NaCl as the pore size decreased. A solution-diffusion model used to analyze this permeation behavior was consistent with a systematic decrease in rejection as a function of porosity. These findings represent the first demonstration of the concept of tuning the selectivity of COF membranes by systematically reducing the effective pore size within a given topology. We are currently investigating new fabrication techniques that offer improved crystallinity and thickness control across a broad range of imine-linked COFs and studying solute rejection as a function of film quality.

MOF thin films offer straightforward access to a broader range of topologies and smaller pore sizes more appropriate for salt rejection from water. However, most MOFs have insufficient stability in water for aqueous membranes. The oxozirconium MOFs are notable exceptions, which led us to explore their synthesis and isolation as thin films. Using a combination of bulk characterization techniques and high-resolution transmission electron microscopy (HR-TEM), we discovered and mapped a complex temperature-topology relationship of MOFs comprised of hexanuclear oxozirconium nodes and tetratopic porphyrin-based linkers. These experiments identified two types of MOFs as kinetic products, as well as a third MOF as the thermodynamic product. The two kinetically favored MOFs, which have notably similar sorption behavior and diffraction patterns, were distinguished by high-resolution transmission electron microscopy (HRTEM) using Pt-modified organic linkers. This understanding of MOF formation informs current work to generate MOF thin films using 2D MOF particles. Zr-2D MOF and Cu-2D MOF particles were characterized by HRTEM, and subsequently used to generate thin films on silicon substrates. The MOF thin films fabricated from Cu-2D MOF exhibited a smoother surface compared to the ones from Zr-2D MOF. We are now focusing on optimizing film-casting methods to generate MOF thin films with fewer defects and controlled thicknesses, which will be used to test their rejection performance of organic compounds and inorganic ions.

NSF Big Idea

Includes

NSF INCLUDES (Inclusion across the Nation of Communities of Learners of Underrepresented Discoverers in Engineering and Science): Enhancing STEM through Diversity and Inclusion: Transforming education and career pathways to help broaden participation in science and engineering. NSF has funded 67 launch pilots to date. The focus of these NSF INCLUDES launch pilots spans a number of broadening participation activities – from STEM engagement and preparatory experiences for students and other community members to educator training to new academic programs that expand access to STEM education.

https://www.nsf.gov/news/special_reports/big_ideas/includes.jsp

SciLinkR: Transforming How Scientists and Engineers Connect with The Public

Brandeis University, Seth Fraden

There is increased emphasis from academic institutions and funding agencies for scientists and engineers to strengthen their engagement with the public, and scientists and engineers are also searching for opportunities to satisfy these expectations and fulfill their personal civic duties. When they communicate with the public, they not only share knowledge, but also increase trust between science and society and increase excitement for science and engineering. This type of supplemental education has been shown to increase students' understanding of scientific concepts and inspire them to pursue future STEM careers. The problems are that it is difficult for scientists and engineers to know where to go and what to do that to make the most impact with the public. To address these issues, the Brandeis MRSEC used the iSuperSeed2 funding to create the social network, SciLinkR.com, an app that matches engineers and scientific researchers directly with the public (e.g. K-12 schools), to provide science education and to promote knowledge about scientific careers.

Launched SciLinkR.com, a social network to promote science
Brandeis launched the beta-site in March 2019 and >230 users have created SciLinkR profiles to connect with other users via the algorithm-based matching system. Additionally, SciLinkR has generated 15 outreach case studies that can be evaluated for impact and effectiveness.

1. SciLinkR's matching algorithm that uses information from user profiles (location, expertise, and personal biography) to suggest new outreach partnerships.

Fig 1. An example SciLinkR profile.

2. SciLinkR's tracking and verification system or, "SciLinkReports", acts as a repository for outreach and engagement following FAIR data principles. SciLinkReports have multiple elements: names of authors, (e.g. the people who contributed to making an event occur, scientist speaker, organizers and public host), affiliated institutions, dates, abstract-length report, audience, identified disciplines, keywords/tags, acknowledgements of funding, references, supplementary materials, and DOI link.

Partnered with other MRSECs, ARIS and Engineering Ambassadors
After the beta-site was launched, users were invited to join the site through MRSEC email notices, in-person forums on the East Coast, an online webinar with MRSEC Education Directors and various articles. Initial feedback from users has been very supportive and the constructive criticism has helped the Brandeis team identify specific ways that the site can be improved and which organizations to partner with in the future. To develop and strengthen the site, the Brandeis MRSEC will continue to partner with the MRSEC Education Network and work with their new partners in the NSF-funded ARIS (Advancing Research Impact on Society) Center and Engineering Ambassador Network.

Pathways to the Workforce 2019
A Workshop in Leadership, Communication, and Professional Competencies

CU Boulder and **UCSB**

Workshop Motivation

In 2018, the National Academy of Sciences reported that in order to prepare students to meet 21st century grand challenges, it is necessary to train them to:

- think in a broad, interdisciplinary fashion
- work successfully within teams benefitting from diverse perspectives.

The Pathways workshop's goals were to bring together a diverse group of students and post-docs in order to address building professional networks, sharpening their oral and written communication skills, and integrating entrepreneurship with their technical knowledge.

This workshop addresses the *NSF INCLUDES* Big Idea around developing STEM talent from all sectors of society. The workshop was organized and implemented through the efforts of MRSEC Education Directors Christine Morrow (CU Boulder) and Dotti Pak (UCSB) and held at UCSB from 13–16 August, 2019.

Participant Information

Workshop participants were recruited from MRSECs and PREMs and students who participated in recent years as REUs at a MRSEC or PREM. Applications, collected in early 2019, yielded a strong and diverse applicant pool. Participants were selected based on their interest in Materials Science, their leadership qualities, and a demonstrated interest in developing communication and entrepreneurial skills. **The workshop was offered at no cost to the participants.** There were 43 participants from 25 different home institutions across the country and Puerto Rico.

Workshop Program

Morrow and Pak researched, planned and organized the program during Fall 2018 and Spring 2019, paying careful attention to recruiting and retaining a diverse group of expert speakers with talks and activities that aligned with the workshop's goals.

Evaluative Feedback

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

Overall, participants responded very favorably to the workshop. Additionally, several students responded both in the survey and in conversations with and emails to Morrow and Pak that they would be interested in contributing to the next workshop program. It is intended to recruit these students to an advisory committee and set up planning meetings for the 2020 workshop with them using an online meeting platform. Two of this year's presenters (Christine Grant, N.C. State and Gary Beall, Texas State) have already expressed great interest in being involved with the next workshop, planned for August 2020 at UCSB.

NSF Big Idea

Harnessing the Data Revolution

Harnessing the Data Revolution: Engaging NSF's research community in the pursuit of fundamental research in data science and engineering, the development of a cohesive, federated, national-scale approach to research data infrastructure, and the development of a 21st-centurydata-capable workforce.

https://www.nsf.gov/news/special_reports/big_ideas/harnessing.jsp

Harnessing the Scanning-Probe-Driven Data Revolution with Machine Learning

Eun-Ah Kim, J.C. Seamus Davis, Killian Q. Weinberger

Cornell University

This project has been focused on machine learning analysis of scanning tunneling spectroscopy data from pseudogap states of high-T_c cuprate superconductors. There is tight feedback between experiment, theory and machine learning. We have shown that machine learning can recognize different types of order in the experimental data, which allows identification of new quantum states [1]. Theoretical analysis that is consistent with the observations provides further insight into the nature of the new electronic states. The results represent a milestone in the development of this new approach to scientific discovery and mark significant progress in two of the NSF Big Ideas: Harnessing the Data Revolution and Quantum Leap. The ability to uncover hidden patterns in modern large-scale and complex data sets should have implications for a range of science that will benefit society.

An array of artificial neural networks (ANN) was designed and trained to recognize different types of hypothesized order hidden in image-arrays recorded from electronic quantum matter (EQM). Fig 1 is a schematic of the approach. These ANNs are used to analyze an experimentally-derived image archive from carrier-doped cuprate Mott insulators. Throughout these complex and noisy data, the ANNs discovered the existence of a lattice-commensurate, four-unit-cell periodic, translational-symmetry-breaking EQM state. Further, the ANNs found these phenomena to be unidirectional, revealing a coincident nematic EQM state. This identification using artificial neural networks points to the dominance of local, strong-coupling physics as supposed to weak Fermi-surface effects – the Fermi surface evolves much over the range of the analyzed data. In fact, strong-coupling theories of electronic liquid crystals are congruent with all these observations.

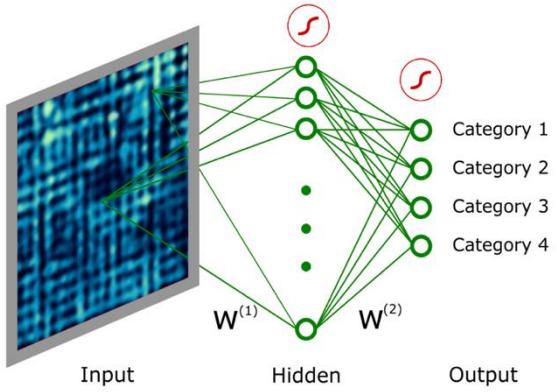


Figure 1. Schematic of ANN analysis procedure for experimental images: the successfully trained neural network with fixed parameters (weights $W^{(1)}$ and $W^{(2)}$ of the hidden layer and the output layer respectively) is a classifier: It classifies each experimental image as belonging into one of the four categories.

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Accelerating Materials Discovery by Data-Enabled Microscopy and Spectroscopy

*An iSuperSEED2 award at the **University of Washington** Molecularly Engineered Materials Center (MEMC)*

David Ginger (Chemistry), J. Nathan Kutz (Applied Math), Jiangyu Li (ME), Xiaodong Xu (Physics)

This award seeks to accelerate the discovery of structure/property relationships – and indeed new materials themselves – by developing and applying new imaging and data science tools in tandem. In our first year of funding, the team has been very successful and has: ***(1)*** expanded the local scanning-probe-based data-science infrastructure while applying these tools to MEMC materials, and ***(2)*** developed new data science methods designed to discover materials physics from image data.

(1) New Scanning Probe Capabilities

We have implemented a new software version of general mode scanning probe microscopy "G-mode",[1] which requires minimal external hardware. Like our earlier methods,[2] G-mode records the entire cantilever displacement vs. time data stream, utilizing post-processing to extract the relevant physics. This approach dramatically increases the information content retained in an SPM experiment. We have applied photoinduced G-mode scanning Kelvin probe microscopy to image carrier dynamics in 2D materials under investigation in IRG1, and observed new phenomena, including charge trapping manifesting as periodic variations in electronic dissipation at early times, perhaps associated with strain in the hexagonal boron nitride layer (Fig. 1A). We have made our G-mode methods available on the publicly accessed Cypher AFM managed by Ginger as part the UW Molecular Analysis Facility (co-located with the MEMC shared facilities), and made our code freely available online.[3]

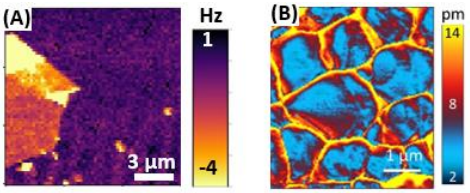

Fig. 1 (A) A sample of WSe_2 imaged via time-resolved microscopy and analyzed via G-Mode, showing contrast with the surrounding hexagonal boron nitride. (B) Linear strain in granular ceria measured via high-throughput sequential excitation microscopy.

We have also developed a new approach called "High-throughput Sequential Excitation" (HSE).[4] HSE combines a series of piecewise sine waves output from an arbitrary wave-form generator on the hardware side, and principal component analysis (PCA) of the digital Fourier transform on the software side, to measure the local frequency response during processes such electrochemical strain, resulting in better stability and higher S/N than previous methods such as dual-amplitude resonance tracking (DART) or band excitation (BE). HSE dramatically increases scanning and data processing speed, and we have used this method to extract local strain data on nanomaterials (Fig. 1B).

(2) New Data Science Tools

Materials can often be described by boundary value problems that are characterized by spatial partial differential equations (PDEs). The spatial dependence of the PDEs model local changes in measured properties, e.g. local stress and/or strain. To date, the governing equations and their local parametric properties are often unknown and cannot be inferred with measurement. Recent advances in model discovery techniques have allowed us to infer governing equations and their parametric dependencies [5] (spatial variability) from measurement data alone. This approach provides a novel mathematical architecture for discovering the physics of materials from emerging data-rich material science efforts. The discovered physics are interpretable and generalizable, helping us learn underlying physical principles and how to manipulate the materials to achieve desired outcomes. The mathematical architecture leverages advances in sparsity promoting regression to down select from a large potential library of governing equations, thus promoting a parsimonious representation of the dynamics. The method has been used for temporal systems, spatio-temporal systems and recently boundary value problems under this grant [6].

[1] Giridharagopal, Precht, Jariwala, Collins, Jesse, Kalinin, and Ginger. *ACS Nano* **13**, 2812 (2019)
[2] Giridharagopal, Rayermann, Shao, Moore, Reid, Tillack, Masiello, and Ginger. *Nano Lett.* **12**, 893 (2012)
[3] "FFTA." https://bitbucket.org/gingerlab/ffta/
[4] Huang, Esfahani, Gerwe, Adler, and Li. Submitted
[5] Rudy, Alla, Brunton, and Kutz, *SIAM App. Dyn. Sys.* **18**, 643 (2019)
[6] Shea, Brunton, and Kutz. In progress (2019)

Universal Chemometrics for Living and Non-Living Materials
iSuperSeed2 Program
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The ability to fingerprint molecular surfaces enables the discovery of key features indicative of life. Additionally, surface fingerprints provide a proxy for material identification and allows characterization of subtle surface changes on cells or abiotic materials. One of the NSF's 10 Big-Ideas is to Understand the Rules of Life. In this regard, our surface characterization elicits chemical fingerprints, at the molecular level, of surfaces to generate patterns for phenotype classification.

The goal of proximity ligation assay (PLA) is to characterize unique surface characteristics and complexity. This complexity analysis will happen by exposing the samples to libraries of ssDNA and sequencing all oligonucleotides that possess a unique interaction with the samples. Proximity ligation of oligonucleotides with sufficient interaction to a sample's surface provides a route for the purification and construction of unique fingerprints.

The libraries we are using have the same forward and reverse primer sequences and only differ in their random regions. Pairs of libraries have been designed to have similar GC content and melting temperature, while their primer binding regions are sufficiently orthogonal where minimal off-target hybridization occurs. The goal is to have 2 ssDNA libraries coexist in the same reaction vessel and ligation only occurs when single-stranded oligos from different libraries are in proximity of each other. We have designed a computational pipeline to generate ssDNA libraries with these properties embedded. Each library consists of 3, 20 base pair regions: a reverse primer region, random region and a forward primer template region.

Once ligation experiments commenced, amplicon contamination became a serious obstacle in the generation of quality data. As additional experiments were conducted, amplicon contamination masked any results from being observed. Thus, we have developed SOPs to limit amplicon contamination from impacting the next iteration of experiments and minimize background ligation of ssDNA. However, these procedures are still influx and constantly being improved.

So far, PLA experiments have been conducted on nucleic acid targets. DNA oligos were chosen as the initial target because DNA hybridization is a well-documented phenomenon that guarantees target-library interaction. Thus, oligo targets have enabled us to characterize and build an intuition on the following experimental parameters: splint concentration, target concentration, library concentration, and amplicon amplification for NGS. The intuition obtained for these parameters will be valuable when we commence to experiment with an array of targets. Another advantage of an oligo target is that we know the sequence of the oligo target. This information can guide us when conducting machine learning and statistical data analysis on sequenced data.

The submission of PLA experiments with DNA oligos as targets for NGS sequencing was a challenge that has been overcome. Due to the length, library design, and library concentrations; it was non-trivial to prep the samples for sequencing. At the current moment, PLA experiments have been successfully submitted to the NGS core and we are awaiting the NGS data. With this initial set of NGS data, we will build predictive models utilizing machine learning and statistical data analysis techniques. The initial models will attempt to reverse engineer the oligonucleotide sequence used as the target.