Harvard University

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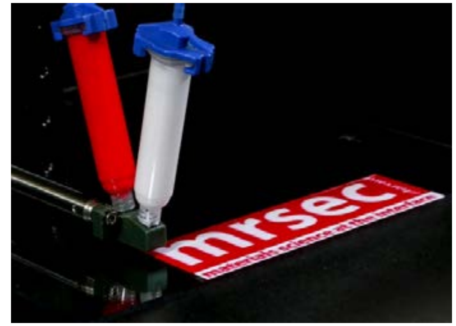
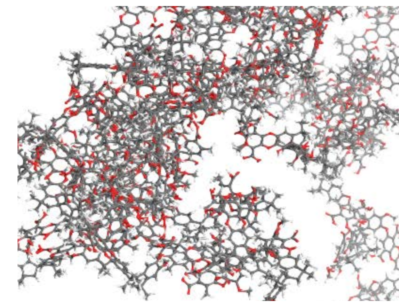
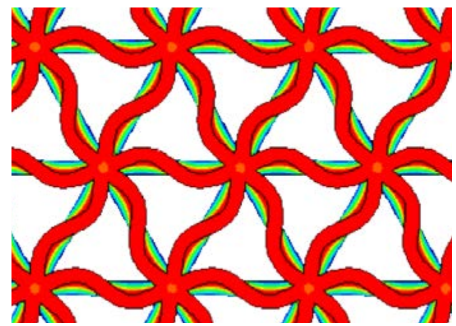
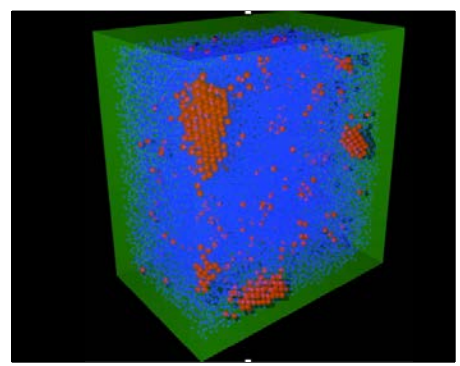
materials science at the interface

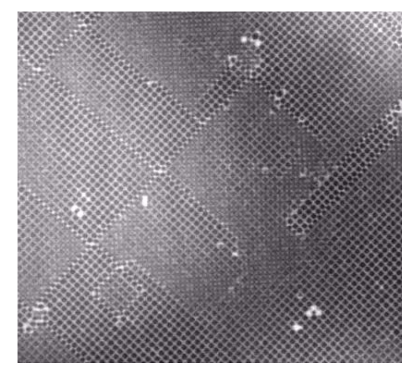
MATERIALS RESEARCH SCIENCE and ENGINEERING CENTER











Director:
Jennifer A. Lewis

Co-Director:
Katia Bertoldi

National Science Foundation
MRSEC
MATERIALS RESEARCH SCIENCE AND ENGINEERING CENTERS

Overarching Goals

(1) Transformational research at the forefront of soft materials science and engineering

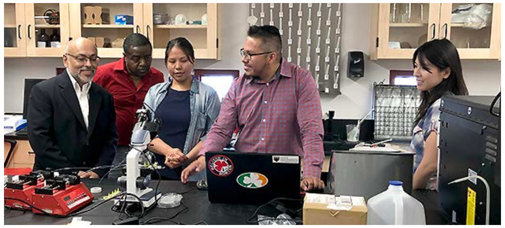
(2) Educate the next generation of leaders within a highly collaborative culture of scientific discovery

(3) Broaden participation in materials science

(4) Engage public in science via soft materials

(5) Translate our scientific discoveries through partnerships with industry and national labs & create high-tech jobs through start-ups

Ideation



Navajo Tech visit

3D printing summer camp

Harvard MRSEC Faculty


Joanna Aizenberg


Ariel Amir*


Katia Bertoldi


Michael Brenner


Federico Capasso


David Clarke


Marine Denolle*


N. Michelle Holbrook


Boris Kozinsky*


Jennifer Lewis


Jia Liu*


Vinothan Manoharan


L. Mahadevan


David Nelson


Kit Parker


Chris Rycroft*


Frans Spaepen


Zhigang Suo


Joost Vlassak


Conor Walsh


David Weitz


George Whitesides

22 faculty members (including 6 new faculty; 5 untenured*)

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Harvard MRSEC Collaborators & Partners

Lucy Colwell
U. Cambridge/
Google

Karen
Crosby
Southern U.

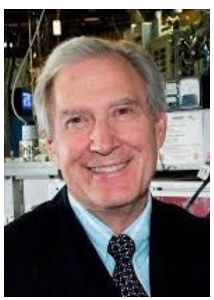
Tarik
Dickens
FAMU

Daan
Frenkel
U. Cambridge

Godwin
Ifere
Navajo Tech

Abraham
Meles
Navajo Tech

Patrick
Mensah
Southern U.



Ron
Pindak
Brookhaven

Subramanian
Ramakrishnan
FAMU

Monsuru
Ramoni
Navajo Tech

James
Rice
Harvard U.

Thiagarajan
Soundappan
Navajo Tech

Richard
Vaia
AFRL

13 researchers from academia, industry, and national labs

Leadership Team

Jennifer Lewis
Director

Bob Graham
Assistant Director

Kathryn Hollar
Education Director

Dave Weitz
Industry Lead

Katia Bertoldi
IRG 1 Lead
Associate Director

L. Mahadevan
IRG 1 Co-Lead

Frans Spaepen
IRG 2 Lead

David Nelson
IRG 2 Co-Lead

IRG 1: Programmable Multiscale and Multi-material Control of Functional Soft Matter

IRG 1 Goal

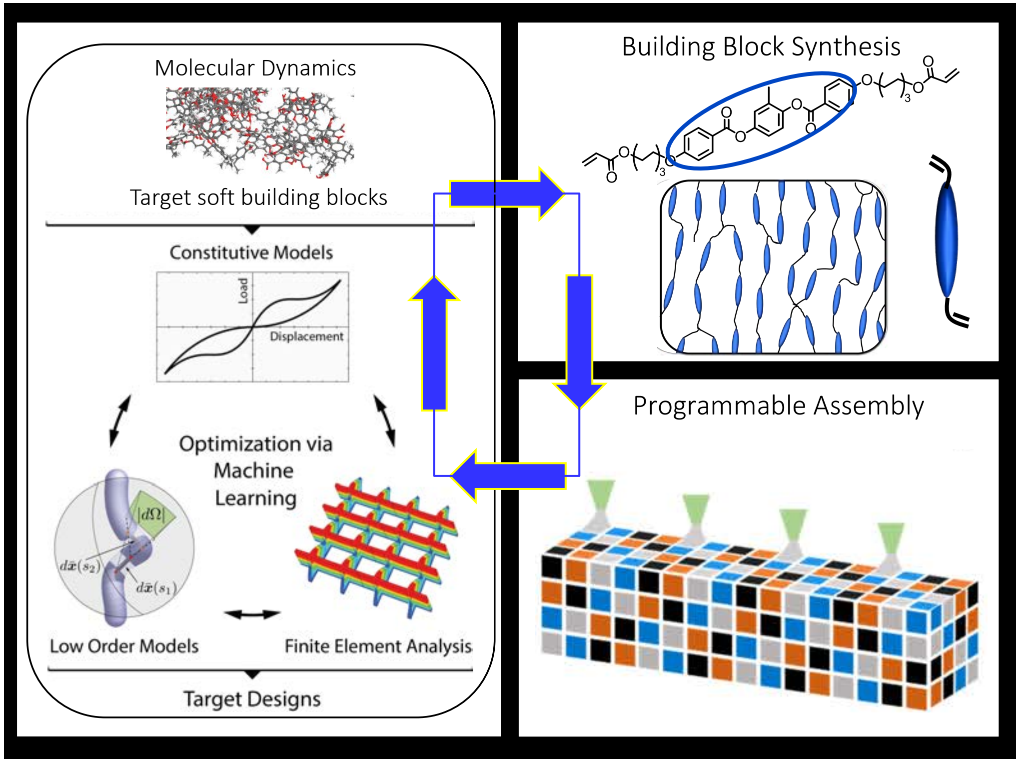
Establish the fundamental design principles to program the multi-scale composition and structure of soft materials with on-demand functionality

Katia Bertoldi
IRG 1 Lead

L. Mahadevan
IRG 1 Co-Lead

Connects to NSF's 10 Big Ideas: *Future of Work at the Human-Technology Frontier*

Tight integration of predictive design, materials synthesis, and digital assembly



3 Research Thrusts

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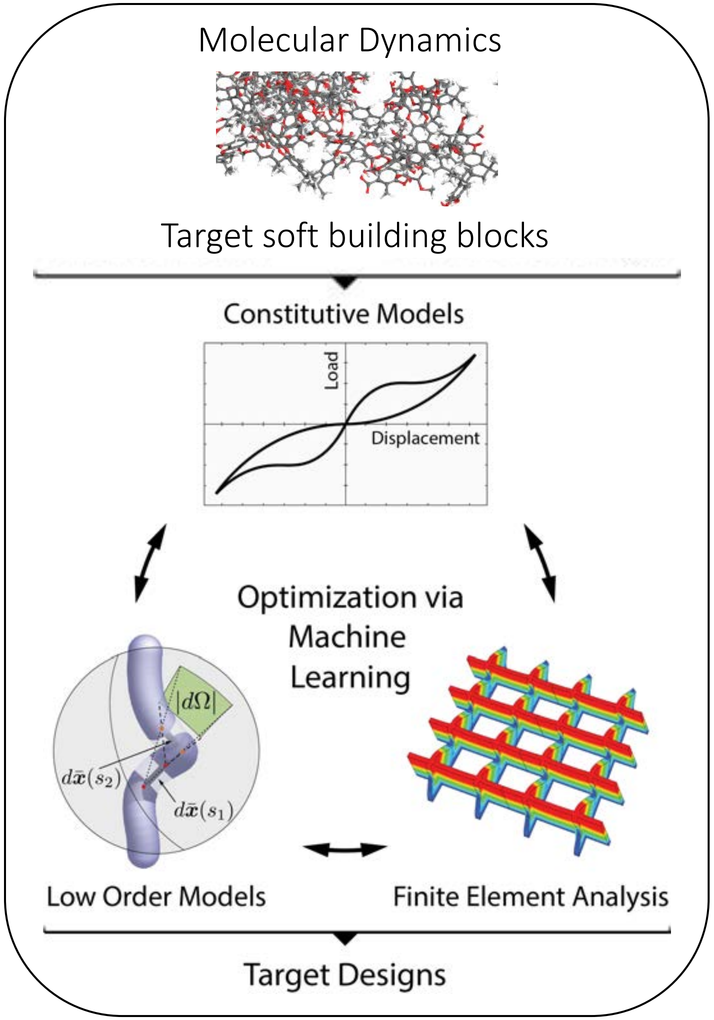
I. Multiscale Predictive Design

Bertoldi, Kozinsky, Mahadevan, Rycroft & Suo



Goal: *Establish predictive design rules* that guide the synthesis and digital assembly of soft functional materials across multiple scales.

Approach: Develop *a suite of analytical and computational models to efficiently explore a vast design space*, identify optimal compositions, and arrangements that give rise to targeted performance metrics in response to external stimuli.

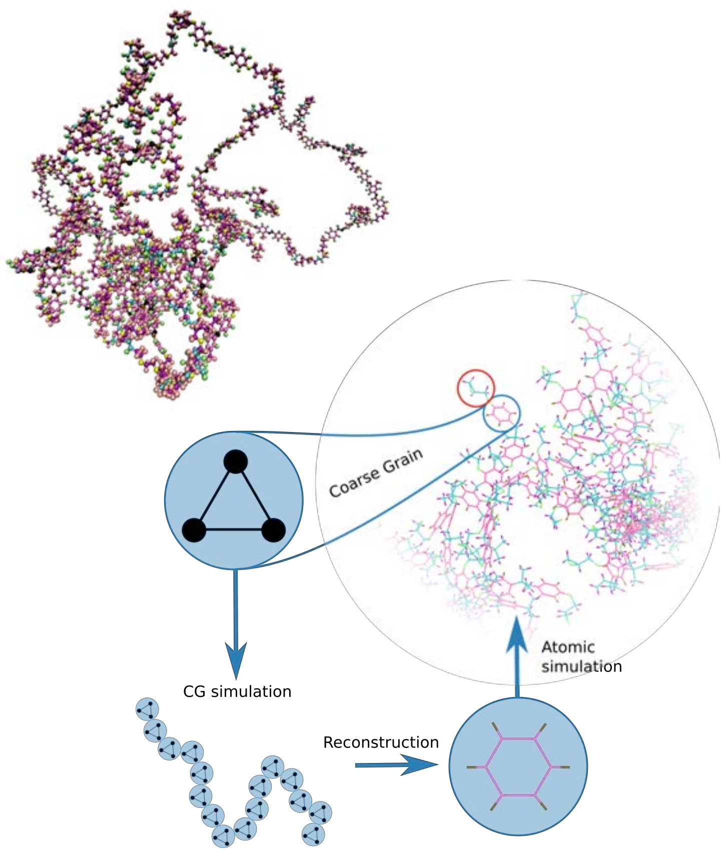
Feedback loop between design and experiments to refine these models & further optimize the targeted functional response (output).

II. Design and Synthesis of Soft Building Blocks

Aizenberg, Clarke, Lewis, Kozinsky & *Pindak (BNL)*

Goal: Understand how *molecular structure* of functional elastomers influences phase behavior, function, and stimuli response.

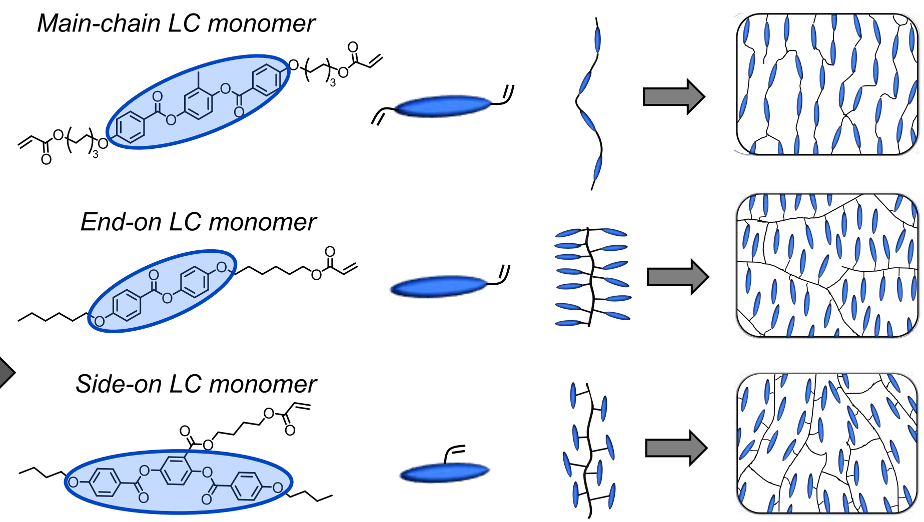
All-Atom MD simulation



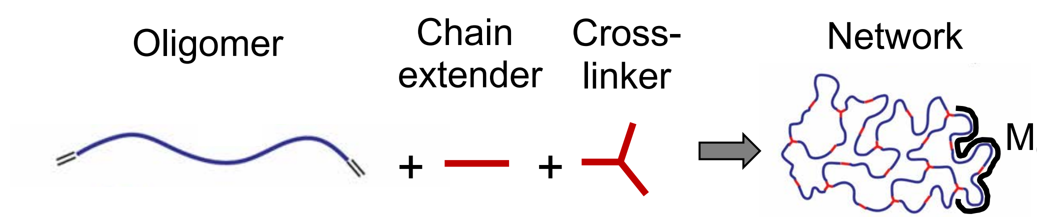
Expand to functional elastomers

(i) Liquid crystal elastomers

Rod-like mesogens | Polymer chains | Network



(ii) Dielectric elastomers

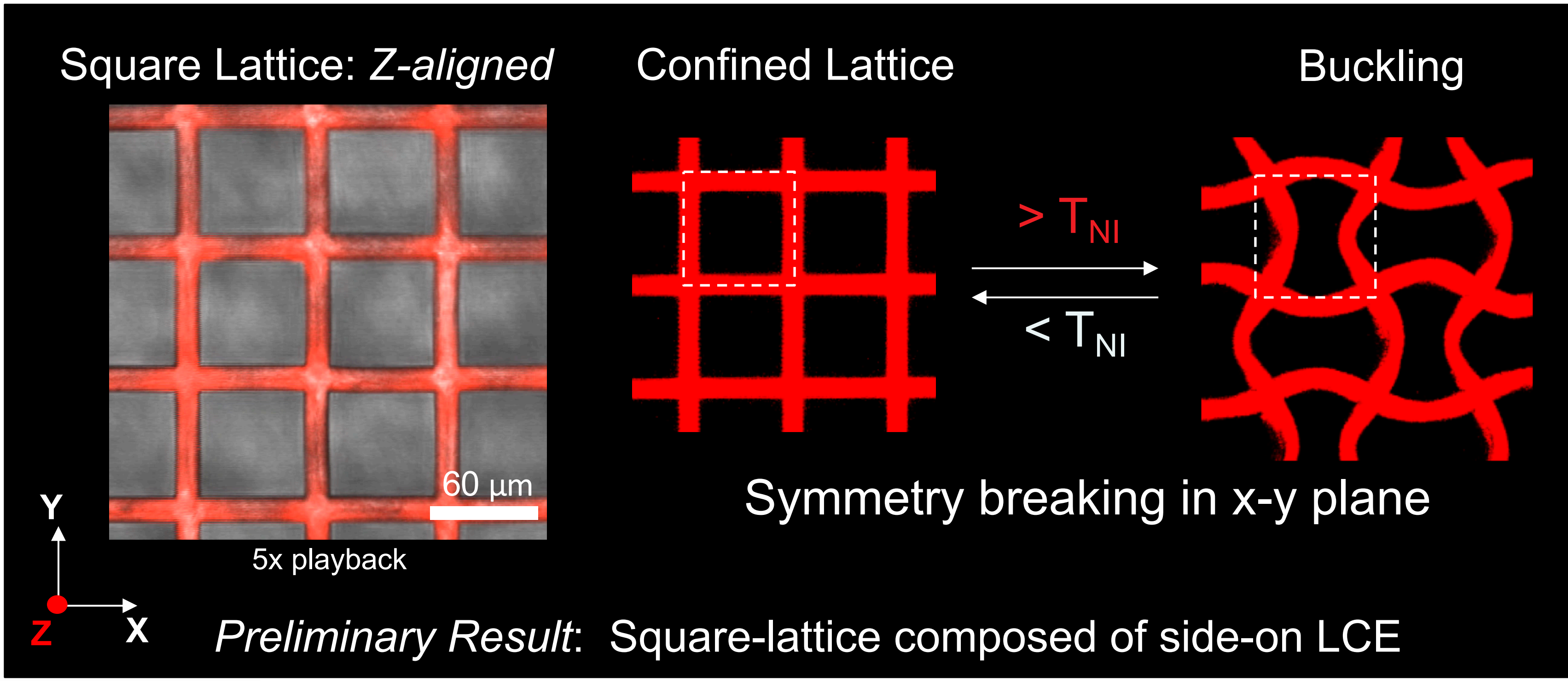


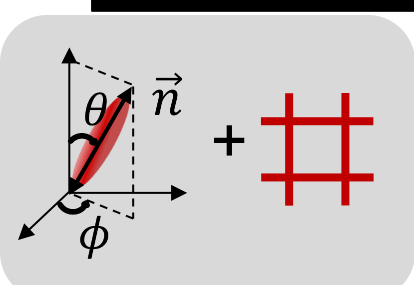
… and functional fillers

Stimuli-Responsive Behavior of LCE Lattices

Aizenberg, Bertoldi, Lewis & Kozinsky

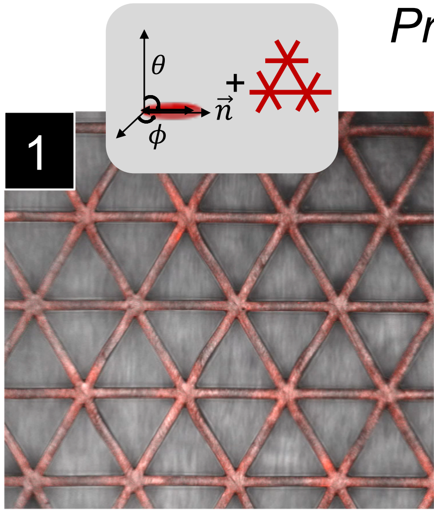
Goal: Understand how *molecular structure* of functional elastomers influences phase behavior, function, and stimuli response.

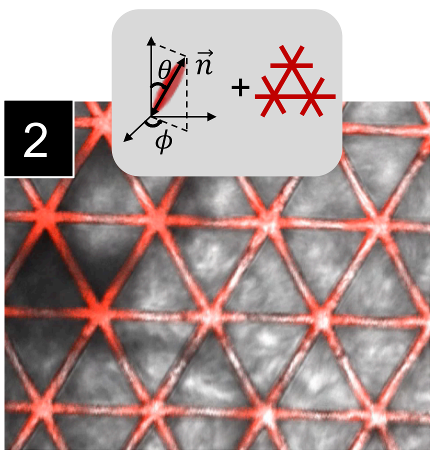




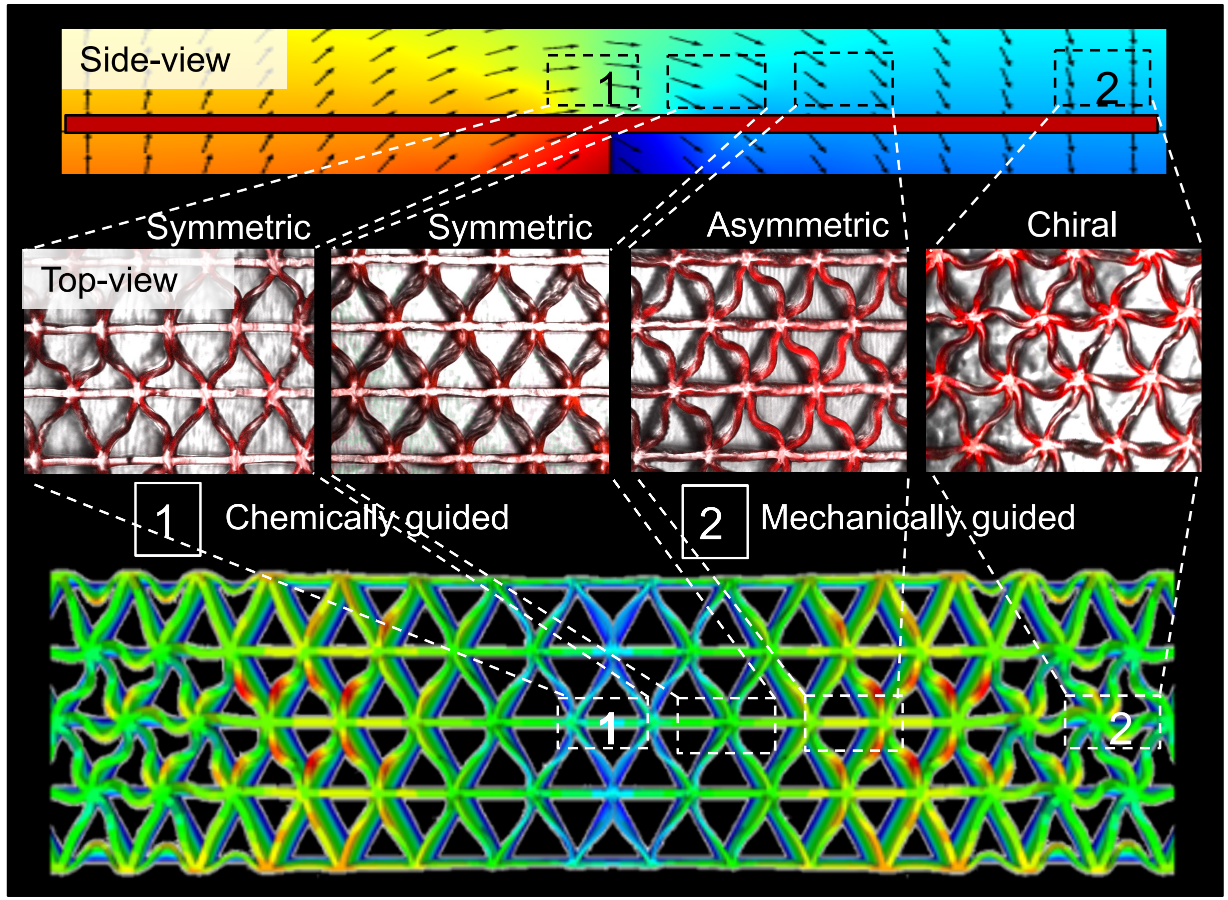
Explore effects of molecular structure, magnetically programmed director alignment & lattice geometry on stimuli-responsive behavior

Side-On LCEs Lattices Programmed in Magnetic Field Gradient





Preliminary Result: Triangular lattice composed of side-on LCE



Complex shape evolution is predicted (FEM) <u>and</u> observed experimentally

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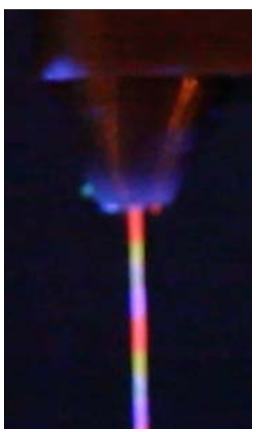
III. Digital Design and Assembly

Aizenberg, Lewis, Mahadevan, Parker & Walsh

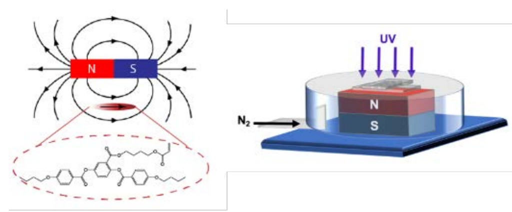
Goal: Create *functional soft matter in 1D to 3D heterogeneous layouts* based on target designs from (I) predictive models and (II) soft building blocks made by controlled synthesis.

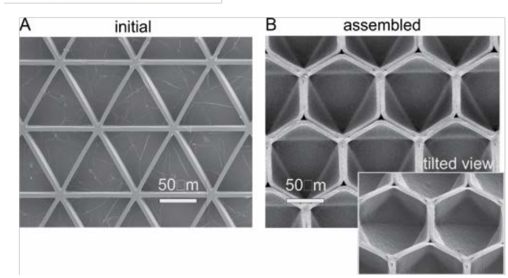
Approach: Use digital assembly methods to *programmably control structure and composition across multiple scales.*

1D Filaments



2D Lattices





3D Architectures

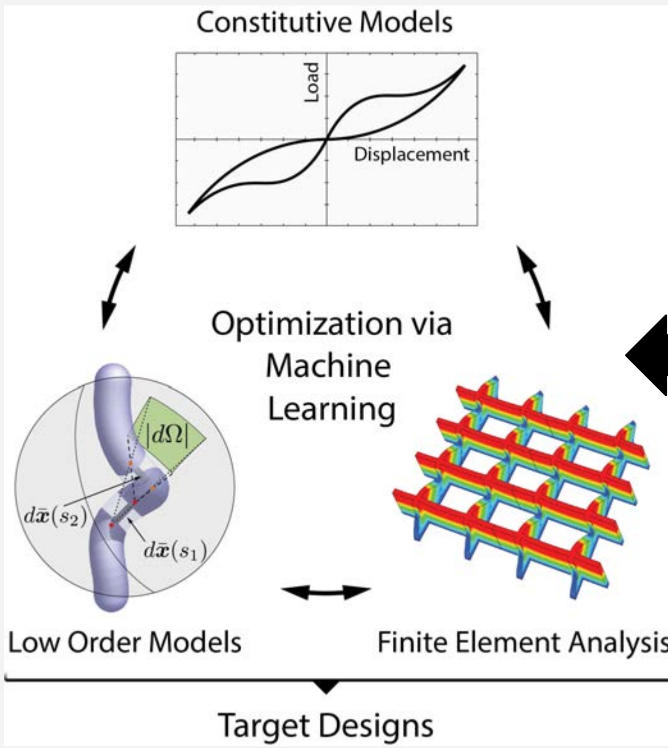
Digital Design and Assembly

Aizenberg, Lewis, Mahadevan, Parker & Walsh

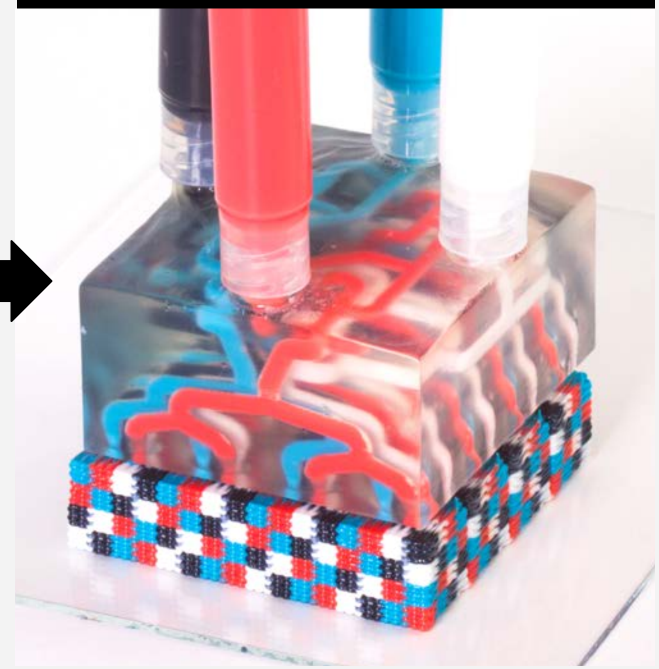
Goal: Create ***voxelated soft matter*** with on-demand functionality

INPUT: Materials, geometric, & functional constraints

Refined models



Digital Assembly

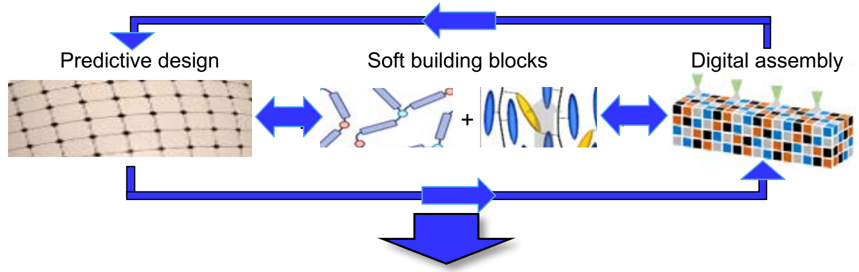


Characterization

OUTPUT: Voxel composition and spatial organization

IRG 1: Expected Accomplishments

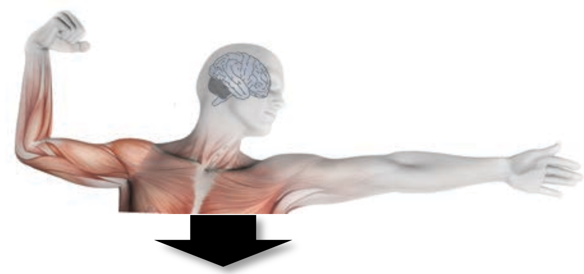
Fundamental understanding needed to program compositional and structural organization of functional soft matter across multiple scales



1) Multiscale predictive models that guide materials synthesis and assembly

2) Functional materials with optimized structure and on-demand response

3) Digital assembly techniques for 1D to 3D voxelated architectures



Functional soft matter for assistive, haptic, and other wearable devices that enhance the human-technology interface

IRG 2: Non-equilibrium Phenomena in Mechanically Soft Systems

IRG 2 Goal

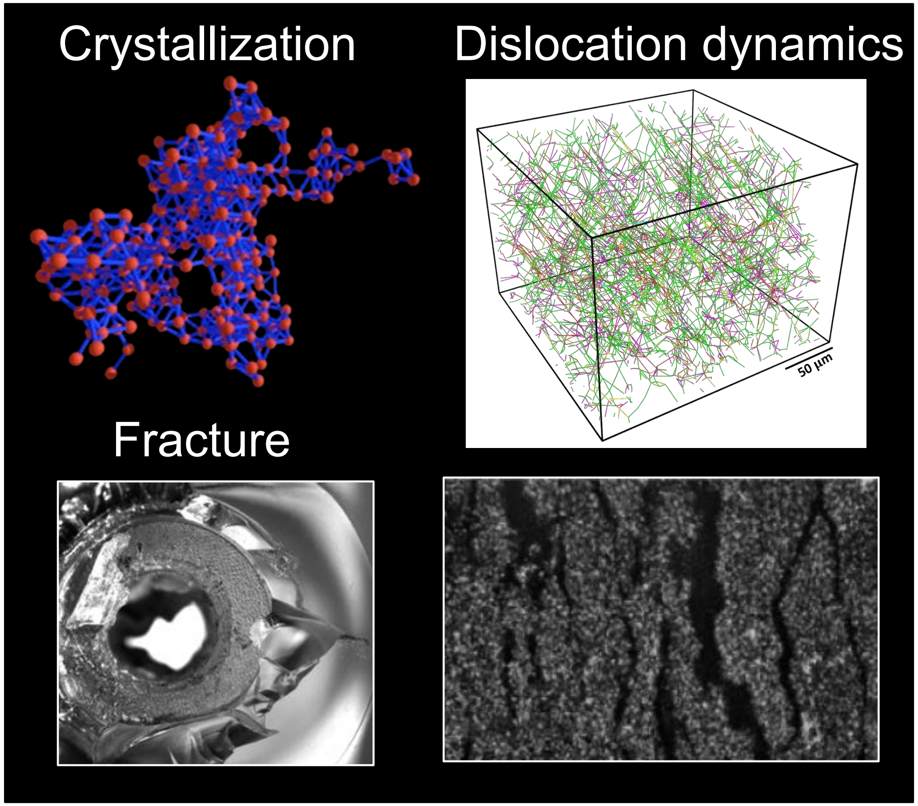
Understand complex dynamics that control crystallization, collective dislocation motion, and fracture of mechanically soft systems

Frans Spaepen
IRG 2 Lead

David Nelson
IRG 2 Co-Lead

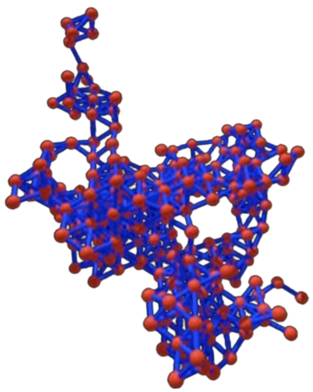
Connects to NSF's 10 Big Ideas:
Harnessing the Data Revolution

Close coupling of data-rich 4D imaging, machine learning, simulations, and theory

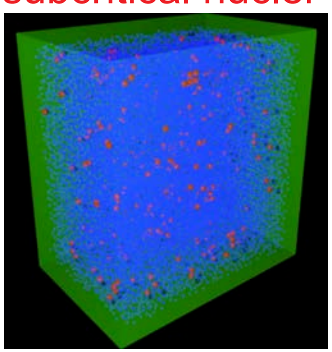


3 Research Thrusts

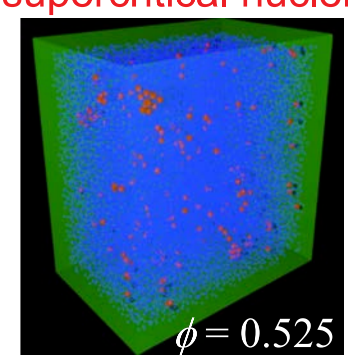
I. Crystal Nucleation



subcritical nuclei



supercritical nuclei



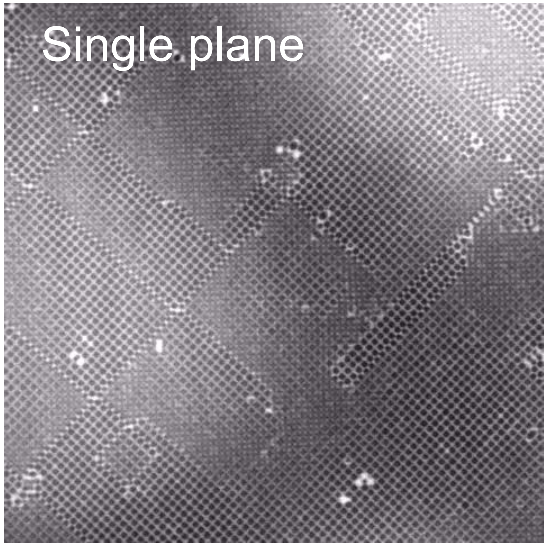
Goal: Understand crystal nucleation *in single and multi-component hard-sphere colloidal systems.* We will use this knowledge to develop new routes for creating atomic scale alloys.

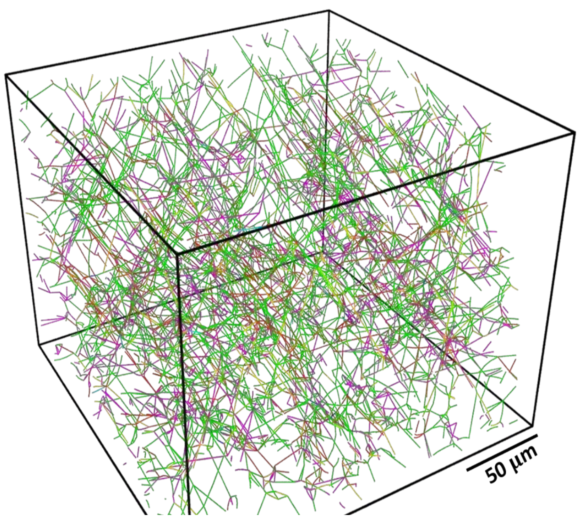
Approach: Colloids can be tailored to model the materials science of undercooled liquids, alloys, metallic glasses, etc., but on length scales 10^4 times larger and time scales 10^{10} times slower, allowing detailed observations of the underlying spatial and dynamical process.

Reduce colloid size from 1μ → 300nm to further enhance particle numbers, 3-4x10^6 and time resolution = 30x. *(Spaepen, Weitz, Whitesides)*

We will complement these observations with expertise on theory (*Nelson*), efficient computer simulations augmented by machine learning (*Brenner, Colwell* – connections w/ Google and *Kozinsky*).

II. Collective Dislocation Dynamics





Green: Shockley partials
Purple: stair-rod locked

Goal: Investigate collective dislocation motion underlying plastic deformation of materials.

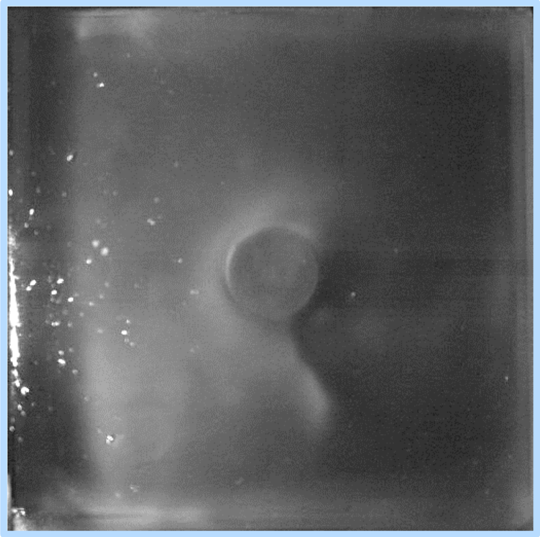
Approach:
Apply shear stress to preexisting dislocation tangle and observe the dynamics of dislocation creation & work hardening.

"…turbulence and work hardening are the two hardest remaining problems in classical physics"
Alan Cottrell

Use data from optical selected area diffraction for colloids to train a neural network to efficiently locate dislocation networks and twin boundaries.

Terabytes of training data for ML!

III. Fracture Behavior

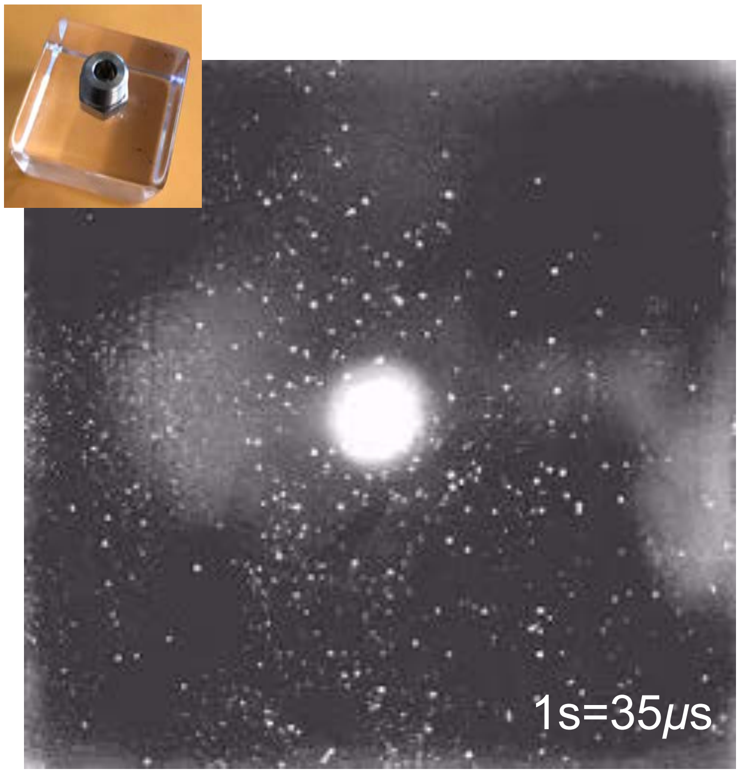


Goal: Explore fracture phenomena in mechanically soft systems to understand their toughening, dissipation, and failure mechanisms.

Approach: Combine high-speed imaging, acoustic emission, and machine learning to develop **new analysis tools** to measure fracture at microscopic to seismic scales.

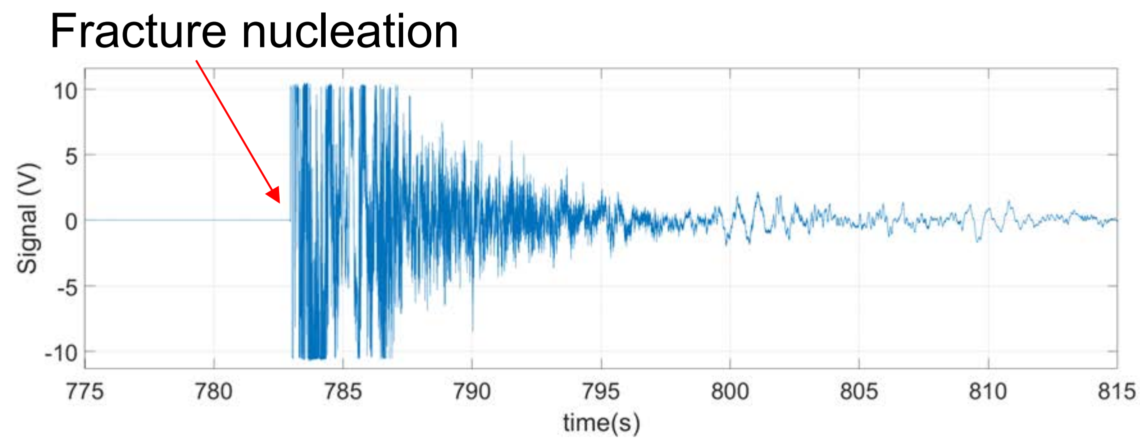
Listening to Fracture

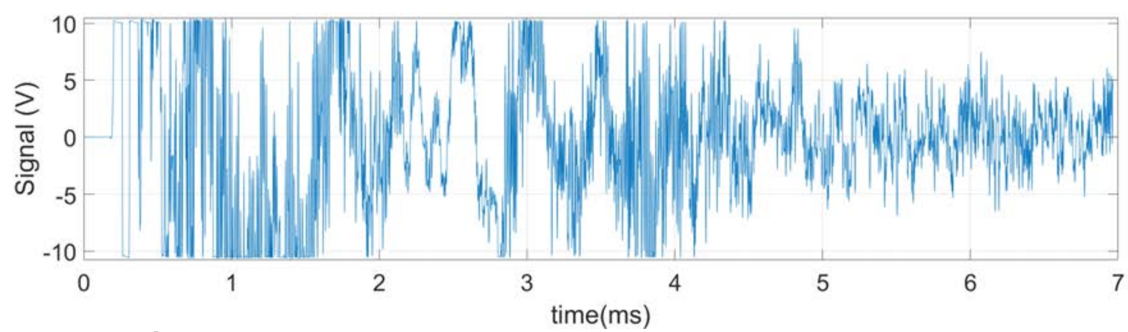
Goal: Combine high-speed imaging, acoustics, and ML methods to unravel hydraulic fracture in model systems.



Sample size: 8 cm

1 cm





IRG 2: Expected Outcomes

- Crystal nucleation and nucleation rate
  – Guide new materials creation and microstructural control
- Fundamental understanding of work hardening
  – Improved modeling of large deformation for processing
- Correlate imaging and acoustics for fracture
  – Predictive tools for acoustic emission from fracture

Exploit big data and data analytics to learn new science

Education, Outreach, and Diversity

Targeted education and outreach partnerships to increase diversity in materials research

Evolving, long-term partnerships
Leadership in recruiting and mentoring
Individual, local, and national impact

Kathryn Hollar

IRG team meeting

REUs

Lecture at Navajo Tech

Strategic Partnerships for Diverse Pathways:
PREM Seed, CREST, Veterans

Navajo Technical University
PREM: K-12 to UG; UG to grad

Florida A&M University
CREST: UG to grad; grad to postdoc

Bunker Hill Community College
Veterans: UG to grad/career

Southern University and A&M College – Baton Rouge
CREST: UG to grad; grad to postdoc

Strategic Partnerships for Diverse Pathways: PREM Seed, CREST, Veterans

Navajo Technical University
PREM: K-12 to UG; UG to grad

Robinson Tom is the first graduate from NTU's BS degree program in biology & will be the first to pursue graduate studies at Harvard U.

TRIBAL COLLEGE
JOURNAL OF AMERICAN INDIAN HIGHER EDUCATION

NTU Biology Graduate to Attend Harvard with Help from NSF PREM Grant

Web Exclusive

Daniel Vandever January 25, 2021

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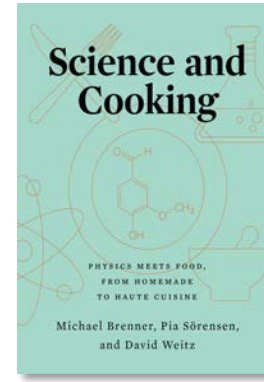
Engage Public in Science via Soft Materials

Science of Cooking

- Public lectures
- EdX course
- New book



Hands-on science camps & workshops for K-12 students

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Industry & National Lab Collaborations

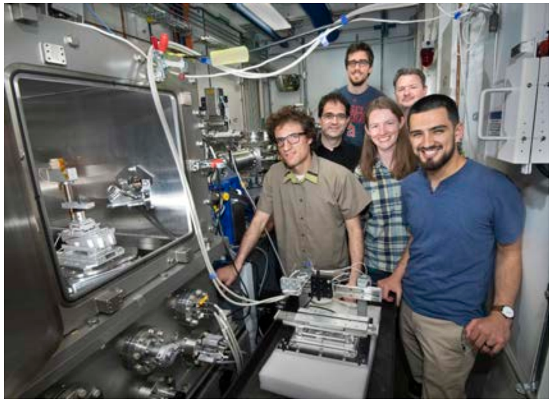
Targeted outreach, national lab and industrial partnerships to increase our impact

Build scientific communities
Leadership in technology transfer
National and international impact


Dave Weitz


BASF Partnership


Sigma-Aldrich Lecture


Brookhaven Nat'l Lab

Summary

The MRSEC is the **heart** of the materials community at Harvard

Together, we will achieve these overarching goals:

- Carry out transformational materials research
- Educate the next generation of leaders
- Broaden participation in materials science
- Enhance public understanding of materials science
- Create new high-tech jobs through start-ups

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Materials Research Science and Engineering Centers