INTERFACING MATERIALS ADVANCES WITH EMERGING TOOLS AND SOCIETAL NEEDS

JANUARY 28, 2021

Chris Hammel (thanks to Jinwoo Hwang, La'Tonia Stiner-Jones and Michelle Richard
(hammel@physics.osu.edu)

Beyond the "10 Big Ideas"

Three questions we seek to address

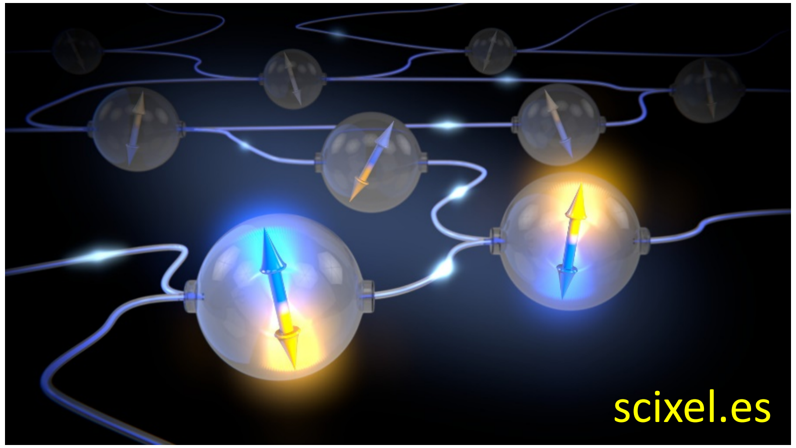
- Opportunities in materials research
  - New Frontier: accelerate massive integration of novel materials into key goals
  - Benefit from MRSEC strengths creativity and productivity through collaboration
  - Continue to diversify and grow universe of partners
- Delineating current impediments such as
  - Access to the rapidly vast materials knowledge universe
  - Diversifying our teams in multiple dimensions
- Impact in materials research
  - Scientific
  - Technological
  - Societal

Tools and Resources: Computational design
High throughput and advanced synthesis/characterization

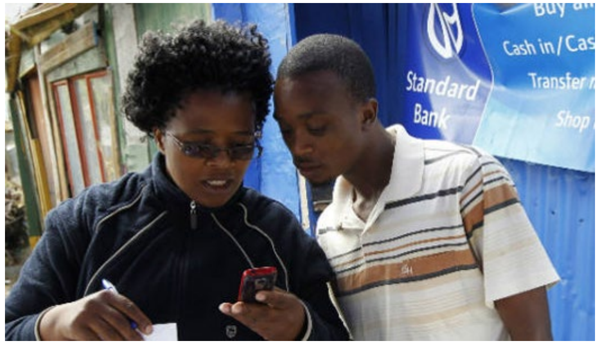
- Materials discovery and design through coupling between materials prediction, synthesis and characterization.
- Computational techniques
  - Electronic structure beyond standard DFT for high-throughput applications
  - Computational infrastructures for data generation
  - Verification and validation for electronic structure databases
- High-throughput combinatorial methods, advanced characterization approaches
- Predicting synthesizability
- Access to this information: Materials databases
  - Materials informatics; development of user interfaces that ease access to materials data

Industries of the Future

- Artificial intelligence (AI),
  - Enhance medicine, security, transportation and education
  - Accessing burgeoning materials knowledge
- Quantum information science
  - Materials research, security, communications
- Biotechnology
  - Health, food security, sustainability
- Wireless communication
- Advanced manufacturing
  - Smart and digital manufacturing, robotics



Opportunities and Barriers



- Broaden the reach of materials for addressing societal challenges
  - Climate change
  - Food security
  - Sustainability
  - Privacy and equitable access to information
- Expanded concept of team
  - Need diverse points of view to identify problems and their solutions
  - Diversity—gender, racial and ethnic, gender identity, age, academic rank, background, disability status—expands ability to imagine and conceive solutions and approaches
  - Computing, informatics, computer science, economics, law, ethics, political science
  - Other research sectors, Air Force Research and Labs, industry
- Barriers
  - Ready, continuous access to state-of-the-art imaging, characterization, fabrication and computation
  - Requires resources
    - Excellence of IRG fundamental science is foundational and must be protected
    - Separate funding: multi-year iSuperSeeds, leveraged MIPs, MRSEC-dedicated MRI

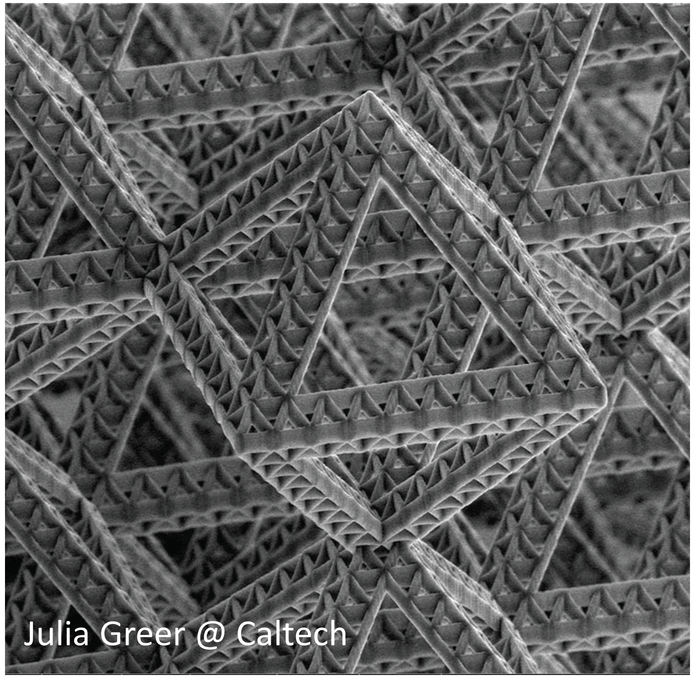
PANEL DISCUSSION

Emerging Frontiers in Materials Research:
Opportunities, Challenges, and Impact

Jennifer A. Lewis

Harvard MRSEC Director
Wyss Professor of Biologically Inspired Engineering

IDEA #1: Voxelated Matter via Digital Assembly



Challenges & Knowledge Gaps:

- Multiscale modeling to predict and validate optimal designs with targeted properties
- Heterogeneously integrating multiple classes of materials
- Real-time feedback and error correction via *in situ* characterization coupled with machine learning

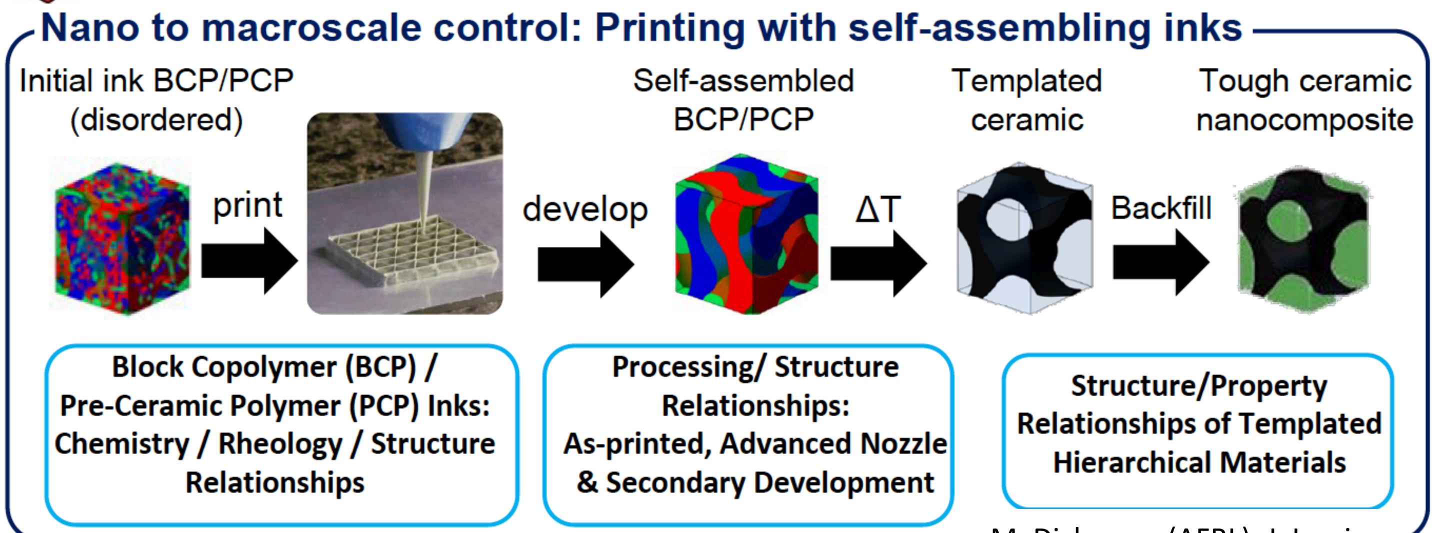
Center effort required:

Multidisciplinary team with expertise in materials chemistry, 3D printing, computational modeling

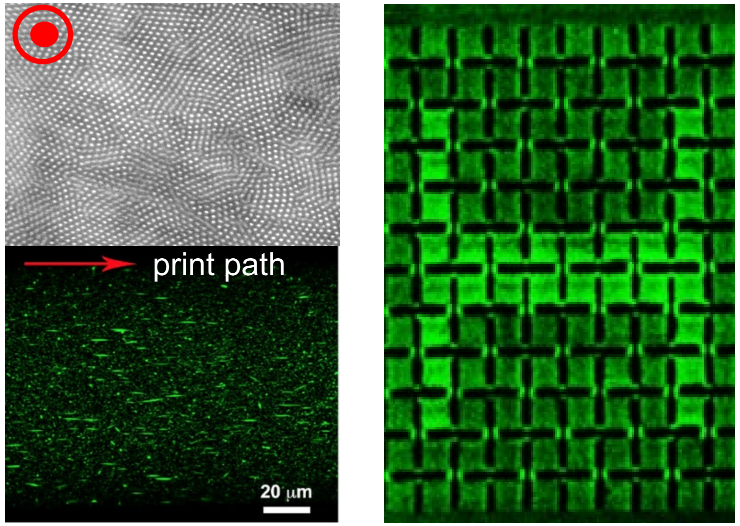
New opportunities: Programming materials composition, structure, and function voxel-by-voxel in 3D enabled by predictive design and *in situ* characterization tools

Impact: New classes of programmable materials with optimized performance

IDEA #2: Merging Digital and Self-Assembly



M. Dickerson (AFRL); J. Lewis



Alivisatos, Yang, Lewis

Challenges & Knowledge Gaps:

- Design and synthesis of self-assembling inks
- What parameters control sub-voxel structure?

  → Need for *in situ* characterization methods

  → Data-driven, multiscale models

Center effort required:

Multidisciplinary team with expertise in materials chemistry, mechanics, functional properties, 3D printing, computational modeling

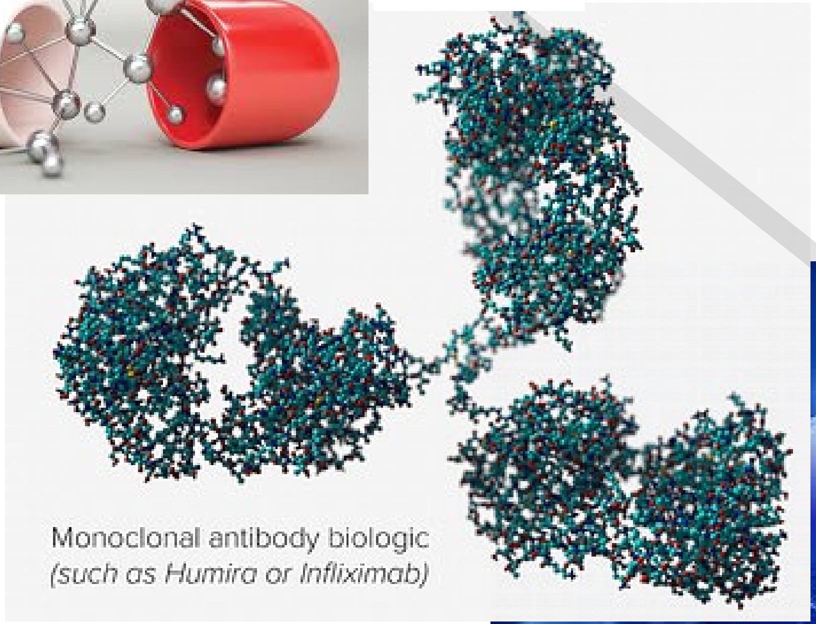
New opportunities: Controlling materials composition, structure, and function at the *sub-voxel scale*

Impact: Nanocomposites for extreme environments and/or multifunctional response

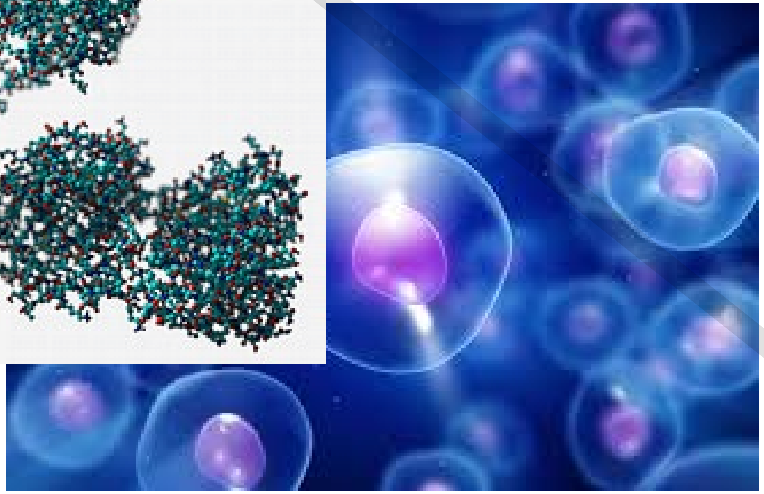
IDEA #3: Biomaterials for Cell-Based Therapeutics

Small molecule drugs

Biologics



Cell Therapies



Regenerative medicine

Challenges & Knowledge Gaps:

- Creating biomaterials that emulating the chemo-mechanical niches in native tissues
- Massively parallel, high throughput methods for assembling cells with biomaterials
- Imaging coupled with AI/ML
- Understanding how biomaterials serve as control algorithms for cells

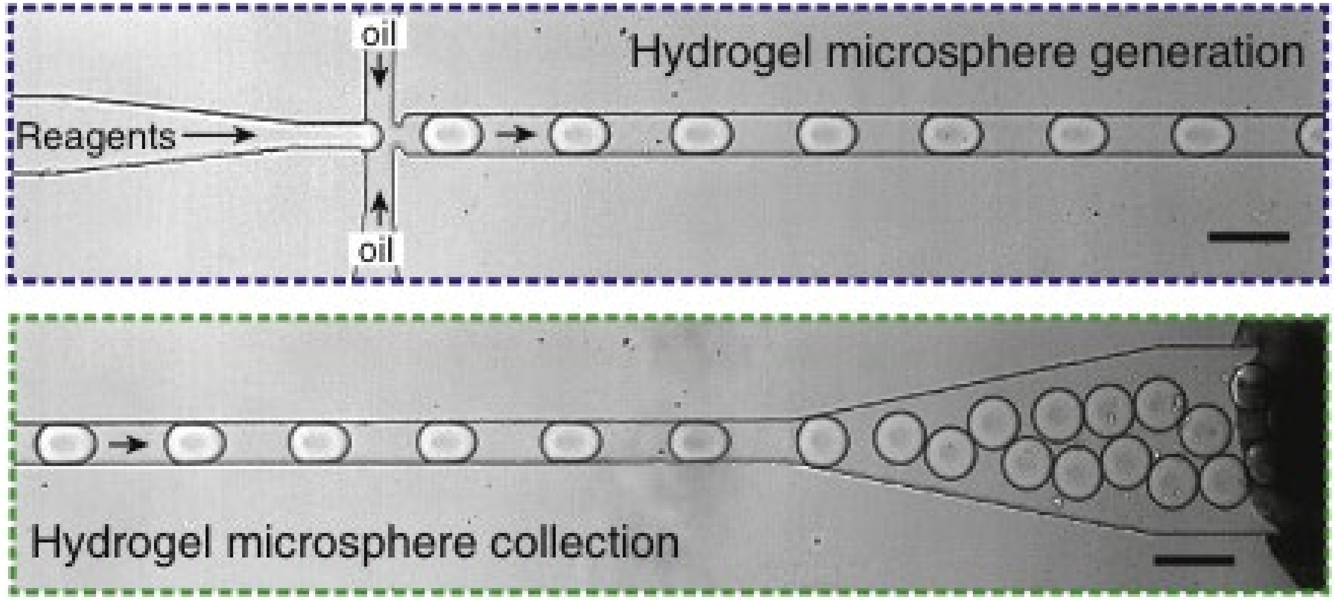
Center effort required:

Multidisciplinary team with expertise in biomaterials, cell biology, microfluidics, imaging, AI/ML

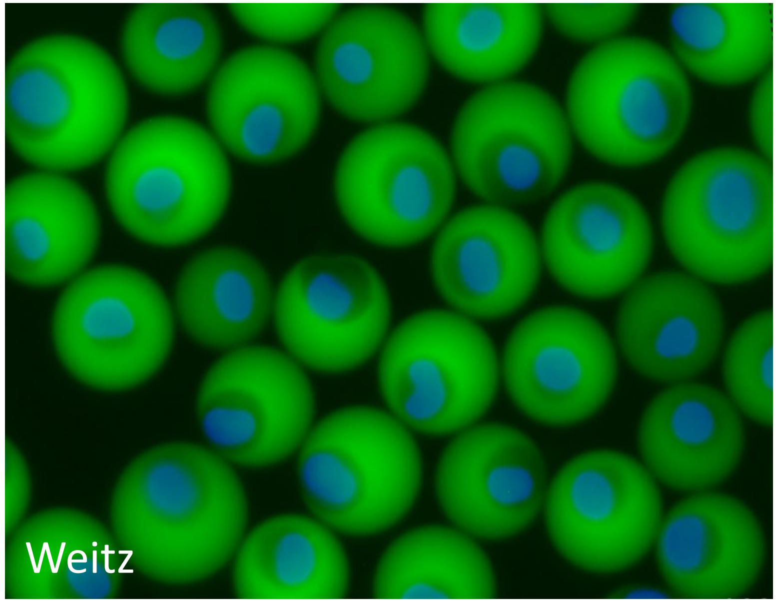
Impact: New cell-based therapeutics that address clinical needs (e.g., cancer, tissue repair & regeneration)

Idea #3 (example): Cell Encapsulation and Control

New Opportunity:
Droplet-based microfluidics for cell encapsulation and high-throughput screening



Impact:
Has already revolutionized single-cell sequencing



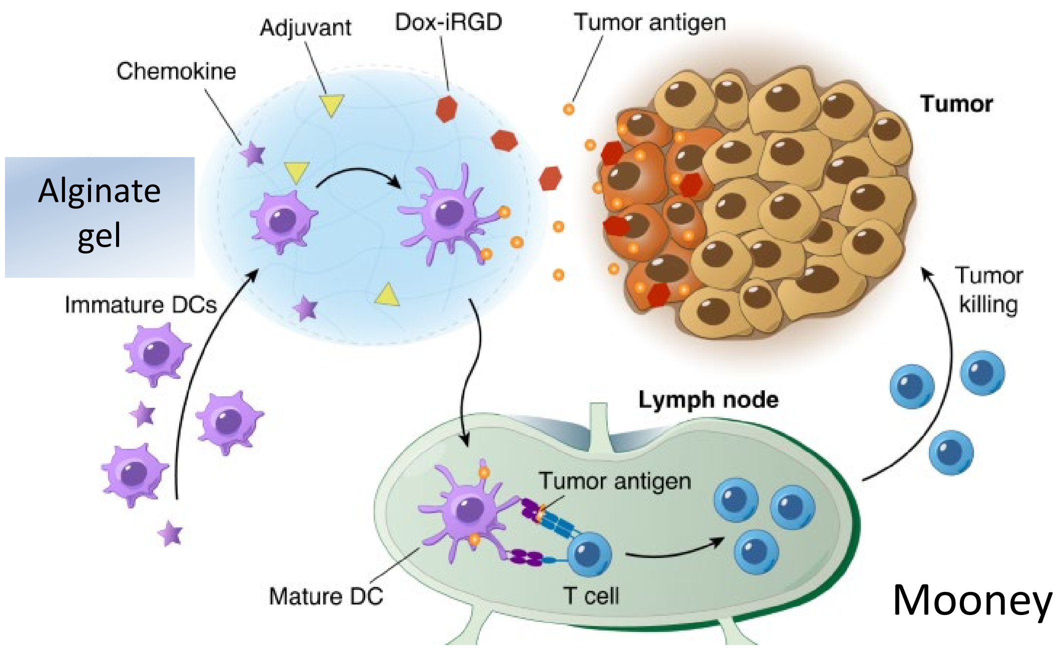
Biomaterials that guide stem cell fate

Combinatorial screening platform for investigating effects of biomaterials (chemistry, mechanics, etc.) on stem cell differentiation, phenotype & function

→ Large data-sets coupled with machine learning methods

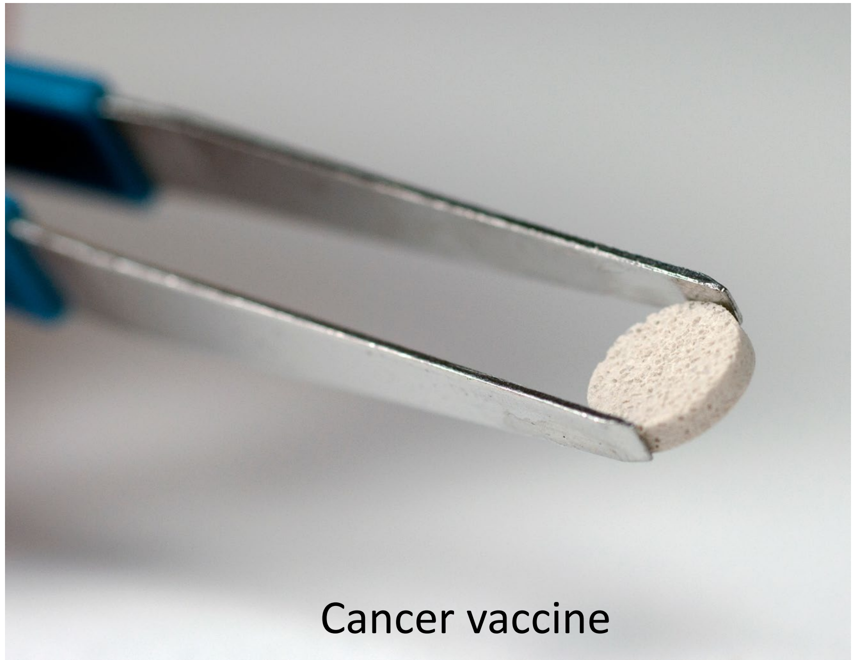
Idea #3 (example): Programming Immune Cells *in vivo*

New opportunity:
Program T-cells *in vivo* via biomaterial scaffold



Mooney

Future impact:
Cancer is one of the leading causes of death in U.S.



Biomaterials that regulate our immune response
Control release of immunomodulatory agents, enhance cell trafficking and function to maximize therapeutic efficacy

Beyond the "10 Big" Ideas
The Return of Manufacturing
The Future of Water

Ram Seshadri (with Chris Bates)
Director, NSF MRSEC at UC Santa Barbara

Thanks to: Michael Chabinyc, Craig Hawker, Tresa Pollock, Rachel Segalman, Susanne Stemmer

Presented virtually at the NSF Director's Meeting, January 28 and 29, 2021

The Return of Manufacturing

President Biden to Sign Executive Order Strengthening Buy American Provisions, Ensuring Future of America is Made in America by All of America's Workers

January 25, 2021

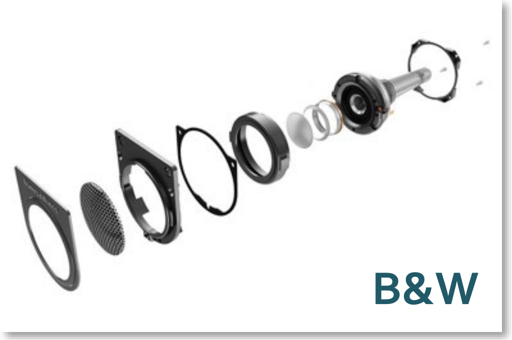
Related January 15th 2020 document from OSTP on *Industries of the Future*

Additive manufacturing (AM) of soft (and less frequently, hard) materials has advanced greatly in structural applications.

Ideal for high value and low–to–moderate volumes

Fundamental science challenges remain:

1. Printing *functionality*, particularly in the hard materials world



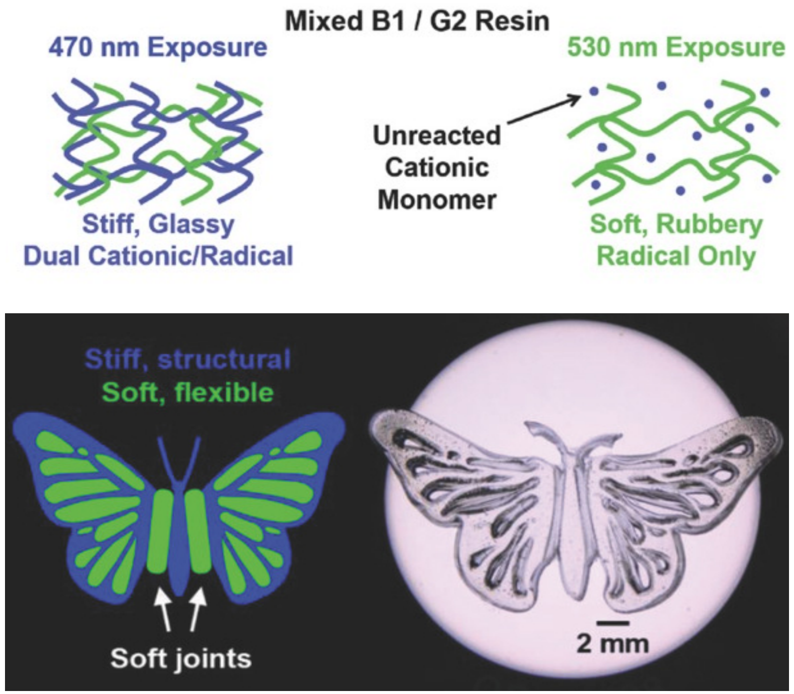
Shaped magnetic fields in a tweeter (not made by AM)

2. AM strategies for composite materials
3. Experimental and computational tools for monitoring processing

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

The Return of Manufacturing

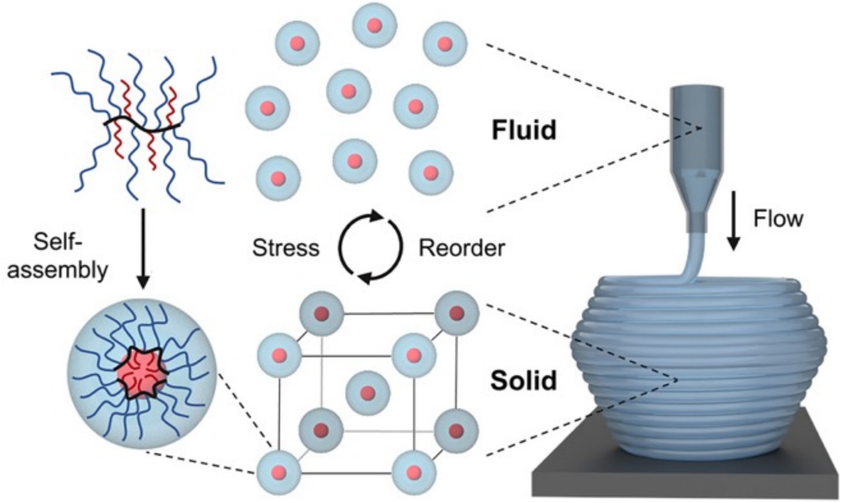
3D objects printed with spatially resolved mechanical and chemical properties



Solution Mask Liquid Lithography (SMaLL) for one-step, multimaterial 3D printing, Dolinskil, Page, Callaway, Eisenreich, Garcia, Chavez, Bothman, Hecht, Zok, Hawker, *Adv. Mater.* **30** (2018) 1800364.

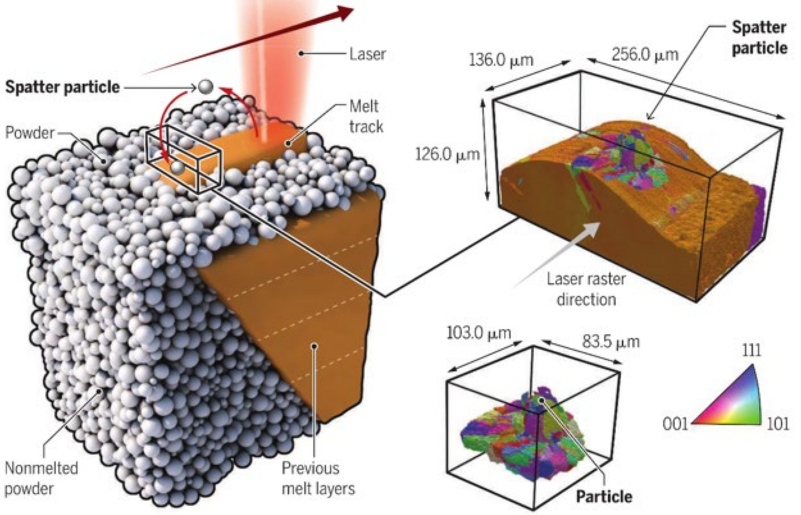
3D printing of soft and solvent-free statistical bottlebrush polymers that self-assemble into well-ordered body-centered cubic sphere phases.

Applications in capacitive sensors.



Room temperature 3D printing of super-soft and solvent-free elastomers, Xie, Mukherjee, Levi, Reynolds, Wang, Chabinyc, Bates, *Science Advances* **6** (2020) eabc6900.

In situ synchrotron x-ray observations of powder dynamics coupled to thermal and hydrodynamic flow modeling to study energy absorption at the scale of powder particles during an AM process.



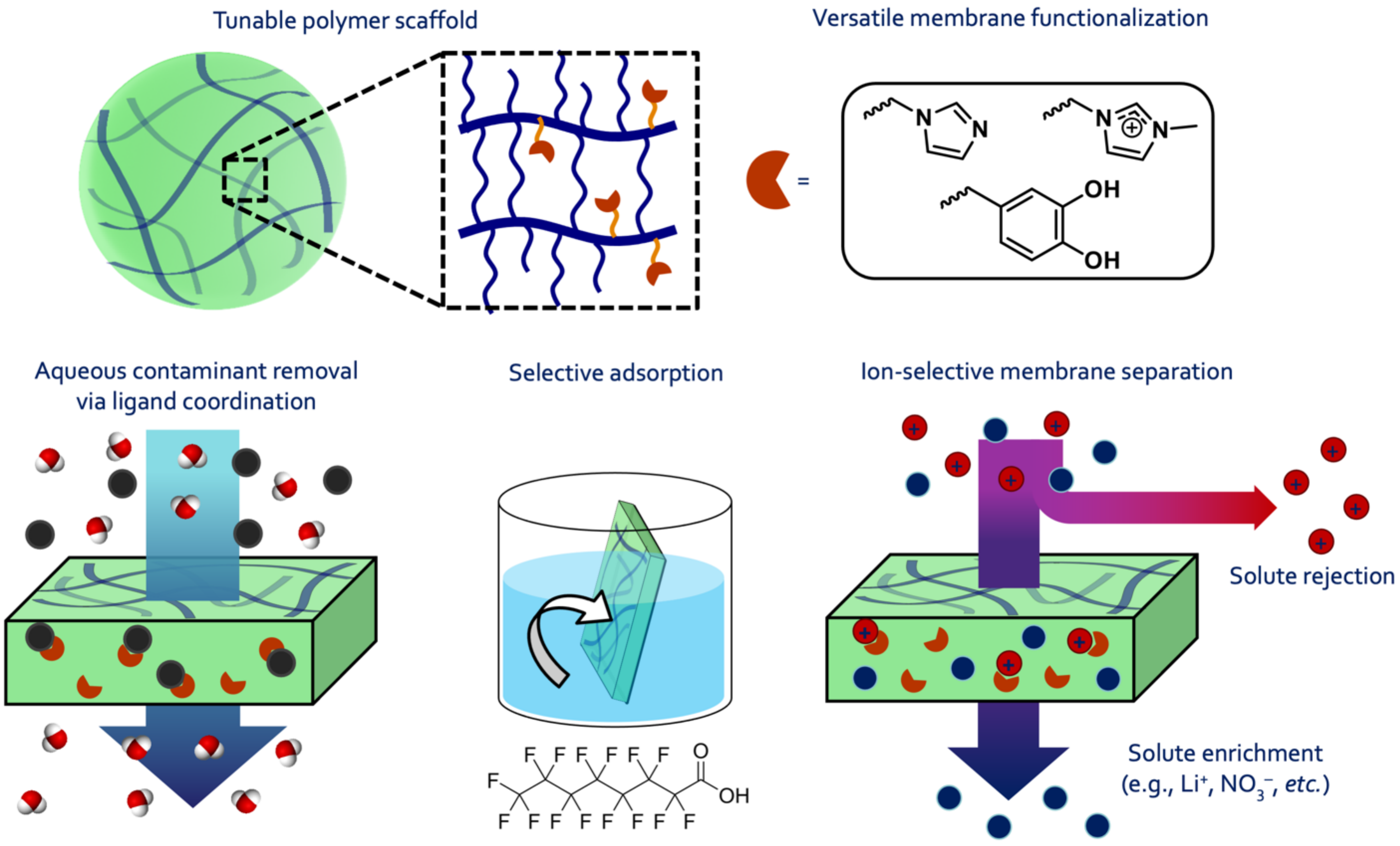
Closing the science gap in 3D metal, Polonsky, Pollock, Science **368** (2020) 583–584, based on Khairallah *et al. Science* **368** (2020) 660–665.

National Science Foundation MRSEC Materials Research Science and Engineering Centers

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

The Future of Water

Fundamental materials advances are still required:



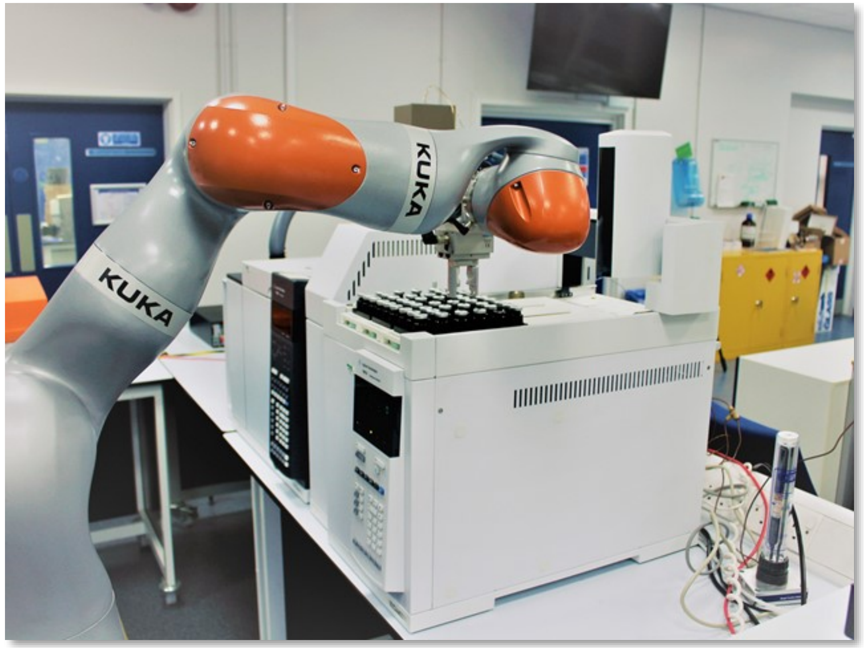
+ use of hydrogels and other slow-release media in agriculture, *etc.*

Thanks to Josh Moon (Rachel Segalman group) for the scheme.

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

Whither US science leadership in materials discovery?

Are we falling behind in innovation?



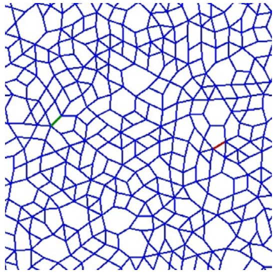
Industrial robots in use in the Materials Innovation Factory at the University of Liverpool [Andrew I. Cooper FRS group]

Particularly apropos during a pandemic.

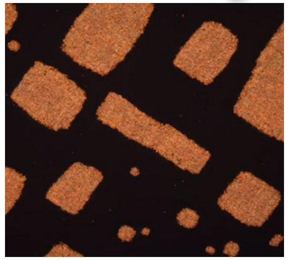
MIPs are a great enabler of science at this scale. We perhaps need more of them? Private foundations?

Margaret Gardel, Uchicago MRSEC

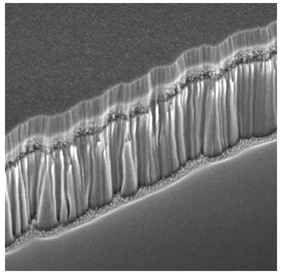
IRG 1:
Trainable Materials



IRG 2:
Active Soft & Living Materials

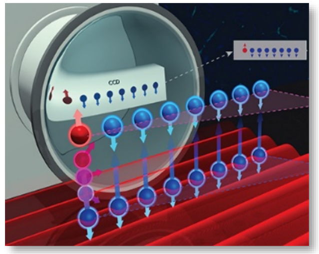


SuperSeed:
Driven Quantum Materials



Rules of Life

Quantum Leap



"BEYOND BIG IDEAS" FOR BIOMATERIALS & BIOTECHNOLOGY

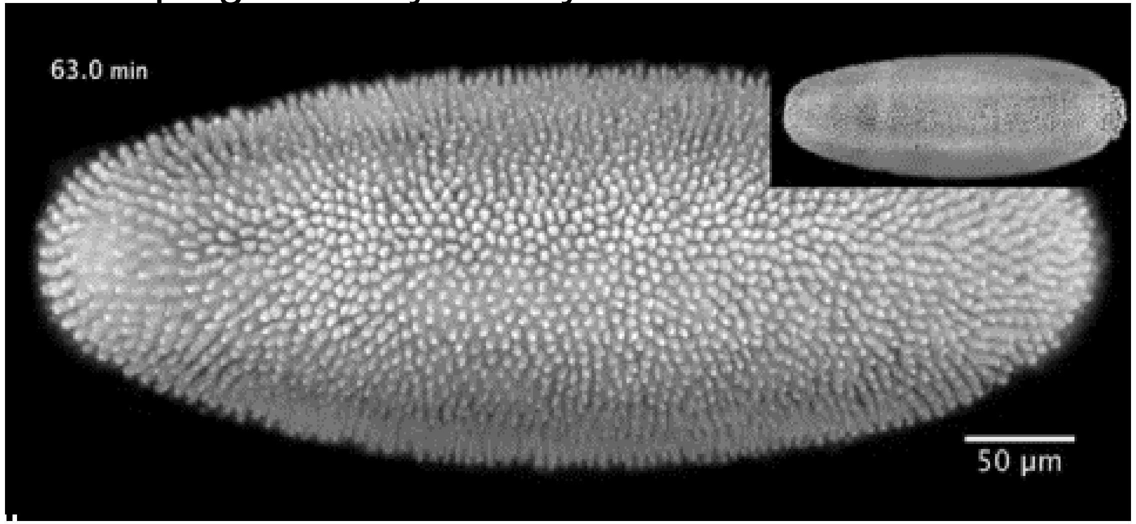
Opportunities in Biomaterials & Biotechnology

Inspiration for Materials Design

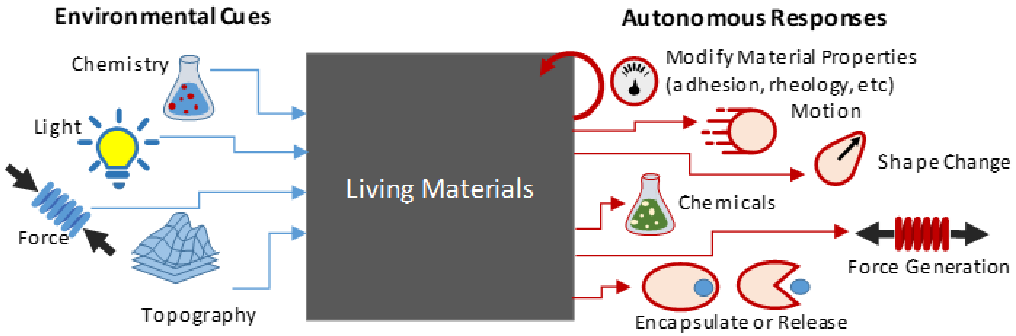
Rules of Life

- Adaptation & Evolution
- Self-Organization & Healing
- Motion and Shape Control
- Sustainable

Developing Fruit Fly Embryo



New Materials: “pluripotent” and “autonomous” materials that could sense their environment and change properties



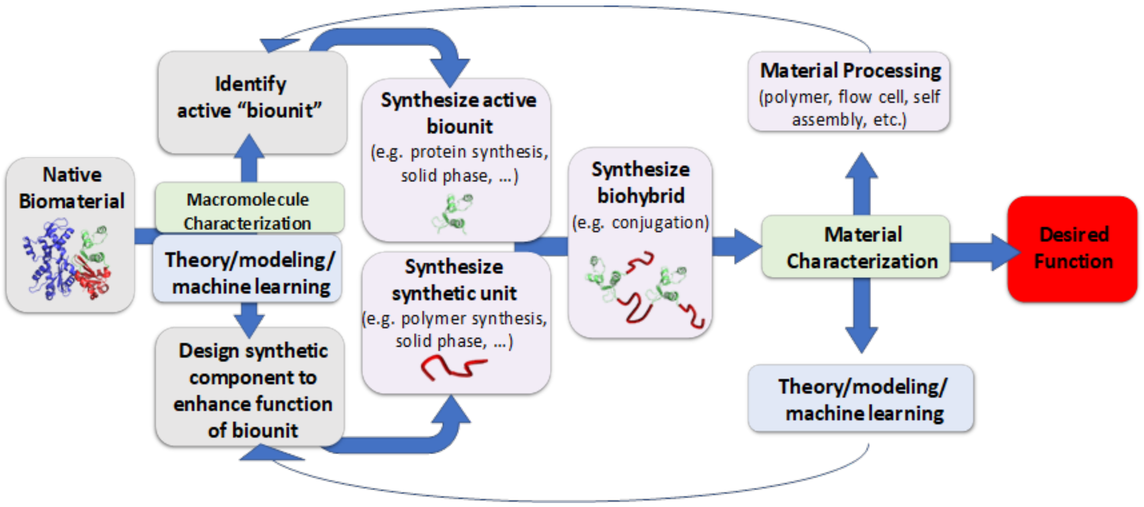
Technology: trainable sensors, actuators and impact absorbers, “lifecycle” materials

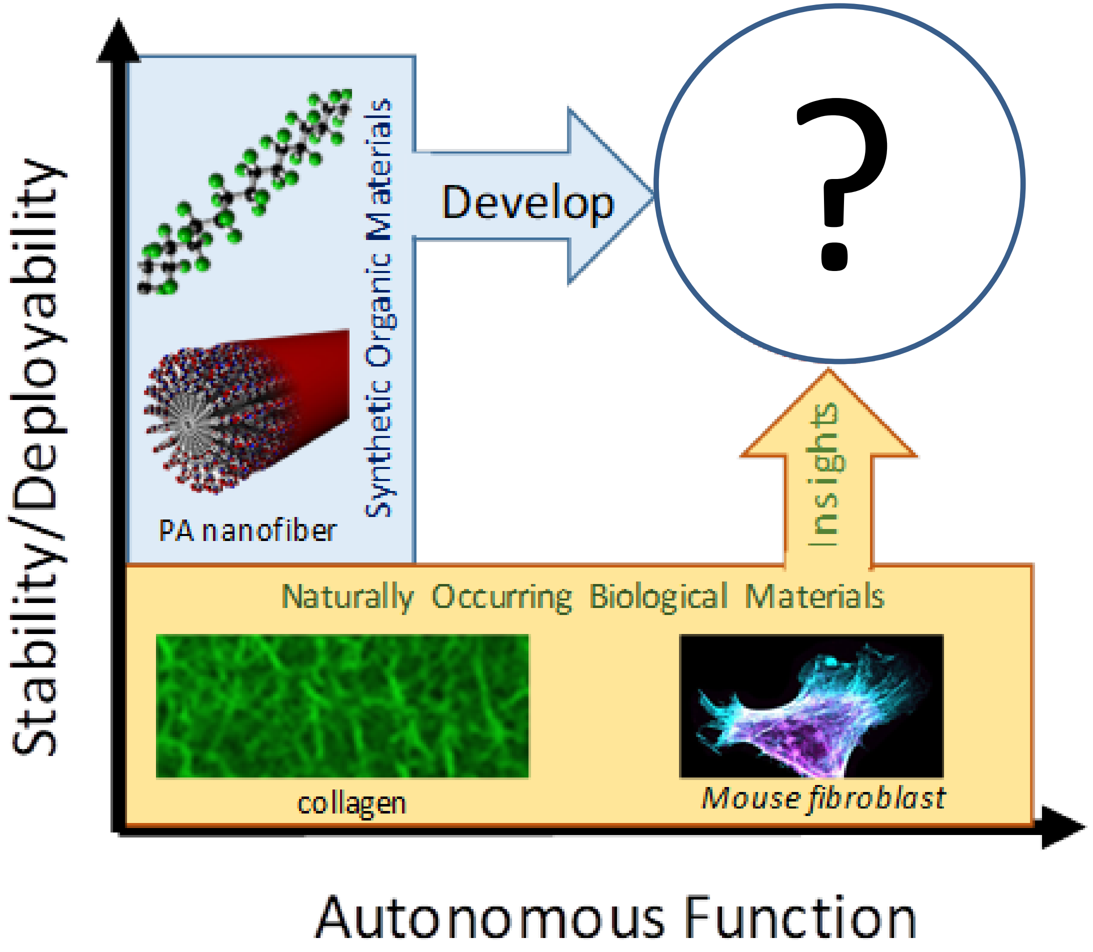
CHALLENGE 1: SYNTHESIS CHALLENGES

NEW BUILDING BLOCKS

- Local force generation
- Reconfigurable bonds
- Actuatable
- Stability & sustainability

Automated synthesis strategies?

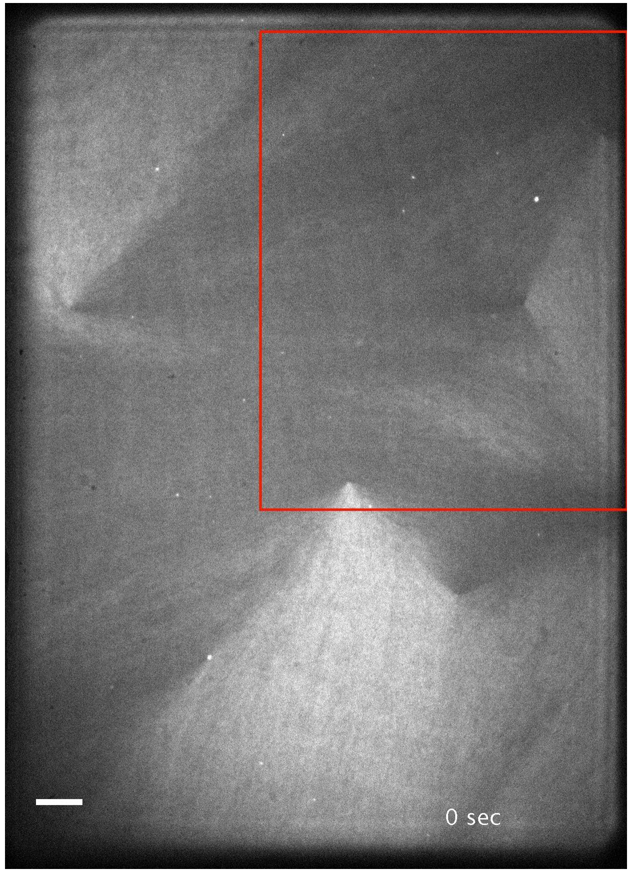


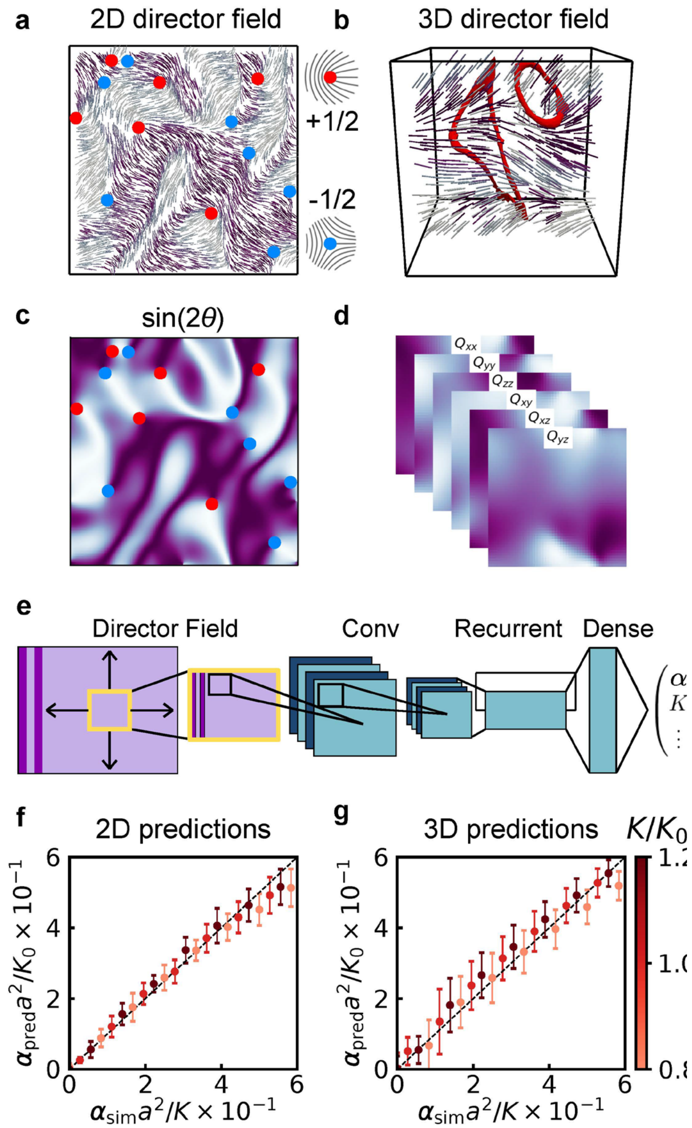


CHALLENGE 2: COMPLEX DATA SETS REQUIRE AI/ML APPROACHES

DATA RICH

- Time-dependent
- Spatial control
- Mechanochemical Feedback





Data Storage & Analysis

Active Learning to inform Experiment and Simulation

Constrain Parameters and Modeling Approaches

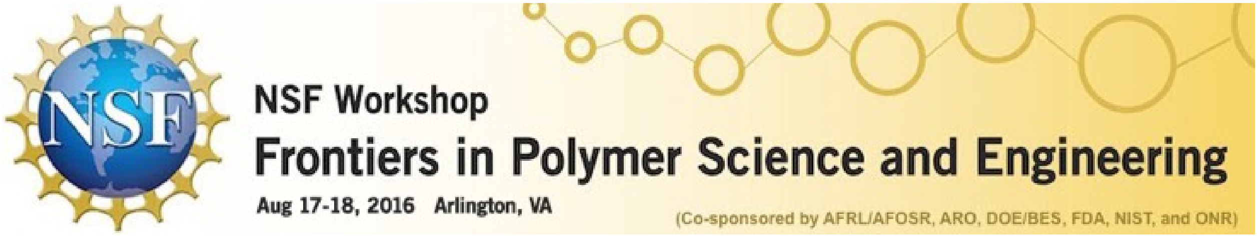
Model Repositories

Macromolecular Materials

Ubiquitous in daily life: plastics, fibers, films, adhesives, rubber, coatings,…

Essential elements of biology: proteins, polysaccharides, DNA, RNA,…

- $500B global synthetic polymer industry (30✕ semiconductors, but comparable to cardboard boxes…)
- Sizeable majority are commodity materials (PE, PP, PS, PVC…) at *ca*. $1/kg
- Increasingly important as valued-added materials (biomedicine, semiconductor processing, Boeing 787, automobiles, membranes for gas separation, fuel cells, batteries, water purification…)
- Value-added properties derive from increased control of both molecular and nanoscale structure
- Advances are increasingly interdisciplinary: requires synthesis, characterization, structure, properties, processing, theory and simuation



https://sites.google.com/a/umn.edu/nsf-polymer-workshop/report

Tim Lodge

21

Bespoke Polymer Materials

Precision synthesis

- Protein-like polymers [*synthetic biology for materials*]
- Sequence control
- Architectural control

Advanced characterization

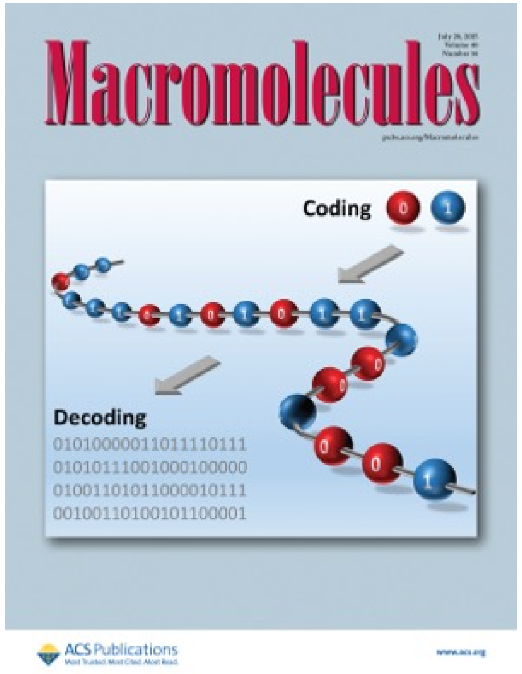
- Molecular characterization: heterogeneity in multiple variables
- Rapid property screening on small samples

Predictive theory

- Parameter space effectively infinite
- Opportunities for artificial intelligence [*machine learning*]

Optimized processing

- Challenge of preserving nanostructure at high flow rates
- Feeds into additive manufacturing [*advanced manufacturing*]



J.-F. Lutz, *Macromolecules* **2015**, *48*, 4759

materials research science + engineering center MRSEC

Sustainable Polymer Materials

Bio-sourced vs petroleum

- 3 days worth is enough
- Too much oxygen, in general
- Requires significant energy input to modify chemistry

New bio-based polymers

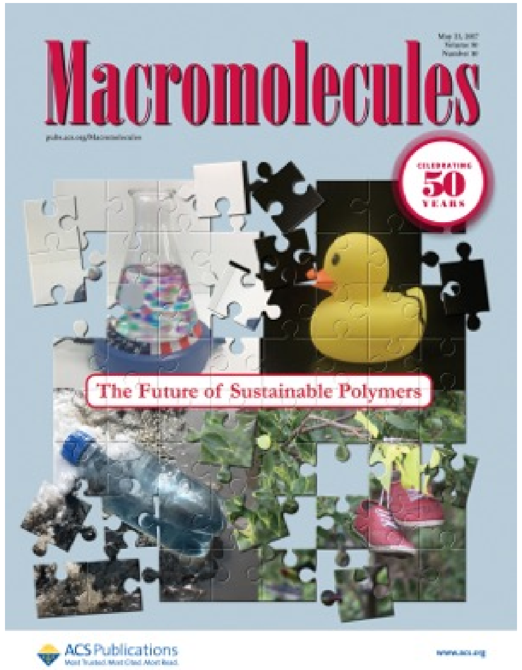
- Will not be price-competitive for commodity use (without regulatory control)
- Will not be property-competitive for commodity use

Need better re-use/recycling strategies

- Degradability for carbon backbone polymers; dynamic covalent bonds
- Blending/compatibilization of mixed streams

Convert biomass into common monomers

- Important strategy, but not a materials problem *per se*



D. K. Schneiderman, M. A. Hillmyer
Macromolecules **2017**, *50*, 3733

23

Additive Manufacturing

Cuts across materials classes

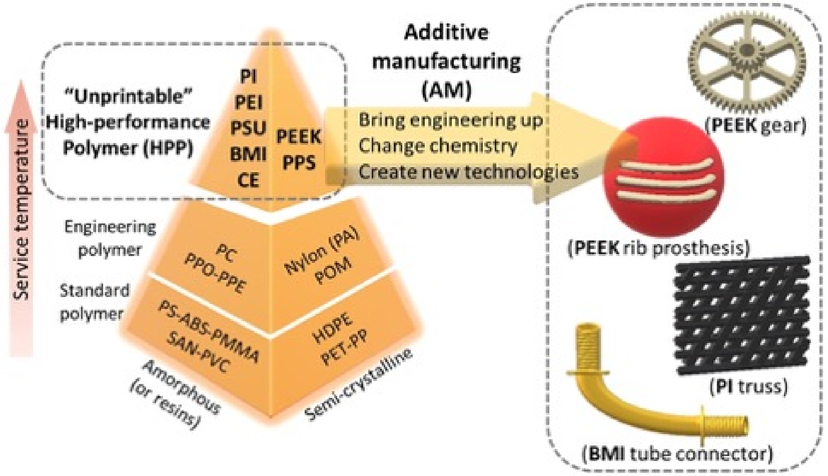
- Polymers, soft materials, metals, ceramics,…

Processing strategies currently ahead of material design

- Need attention to linear/non-linear rheological response
- Diverse solifidication strategies
- Speed is of the essence
- Need modelling/materials feedback loop

Opportunities for hierarchical structure

- Self-assembly (bottom-up) combined with top-down
- Produce/preserve nanostructure on macroscale
- “4D printing”



Boydston, Cui, Lee, Lynde, Schilling *ACS Macro Lett.* **2020**, 9, 1119

materials research science + engineering center MRSEC

Beyond Big Ideas…

National Science Foundation
MRSEC
Materials Research Science and Engineering Centers

What versus How

Prescriptive: do this
Proscriptive: not that

Liberating
Dynamic

Research in a given area or following a given theme, implicitly excluding creativity that reaches beyond our current imagination.

Team-scale research that is fluid and trans-disciplinary. “Bell Labs reborn”

Beyond Big…

MRSEC is not What

MRSEC is *How*

Team-level, sustained over time, dynamically adaptive.

Beyond Big…

Deliberately capacious thematic research umbrellas coupled to high expectations for management practices that foster creative discovery **and that can generalize and scale**.

Beyond Big…

Seek transformative innovations in *research management* that are **agile**, **frictionless**, **adaptive**, and that **collapse distance** in space, time and between disciplines.

Recognize that transformative creative scientific advances are definitionally unforeseeable, yet they can nevertheless be fostered through advances in research management practice and culture. And MRSEC is an ideal hotbed for this.

Beyond Big…

National Science Foundation MRSEC Materials Research Science and Engineering Centers

Thematic research umbrellas:

Material Platforms for Quantum Information Science

Enabling Materials for Sustainable Earth Systems

Materials Discovery informed by Deeply Connected Data

How will you innovate *frameworks of discovery* in this domain?