Materials Genome Initiative & Materials Innovation Platforms

Cosima Boswell-Koller, Ph.D.

Program Director: MRSEC, MIP, and NaFI

NSF Division of Materials Research

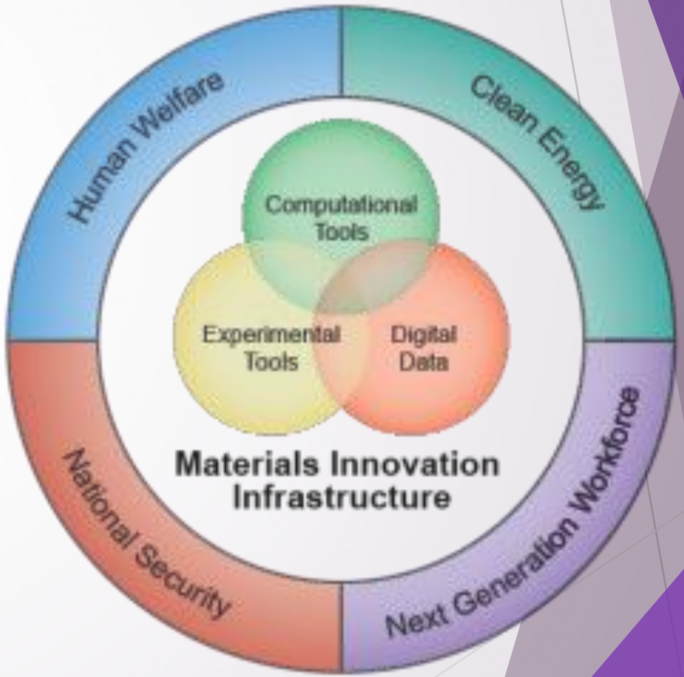
MRSEC Director's Meeting
January 19, 2023

Materials Genome Initiative (MGI)

Established June 2011

Vision:
Materials innovation
is integral to core national needs

Approach:
Accelerate materials innovation through a *Materials Innovation Infrastructure* (MII)



Materials Genome Initiative (MGI)

MGI Strategic Plan 2011 (MGI 1.0)

1. Integrate experiments, computation, & theory
2. Make digital data accessible and useful
3. Develop materials workforce for academia & industry

NSTC Subcommittee for MGI

Co-chair

L Friedersdorf
OSTP

Co-chair

J Christodoulou
ONR (retired)

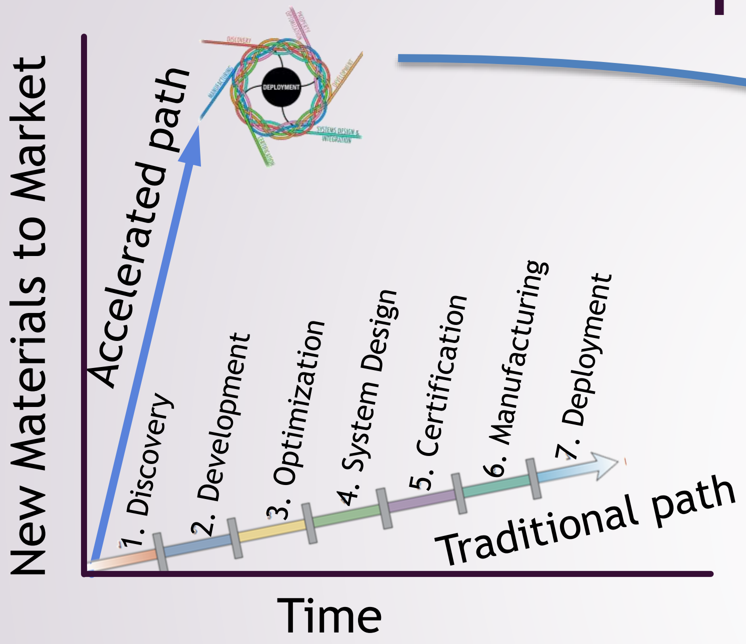
Co-chair

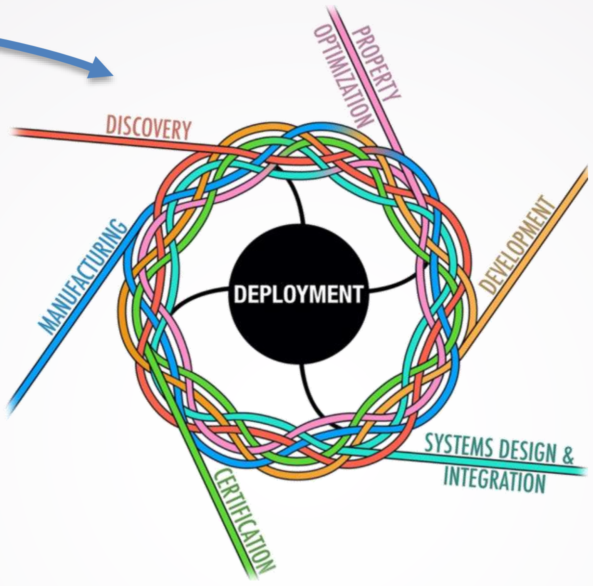
L Sapochak
NSF

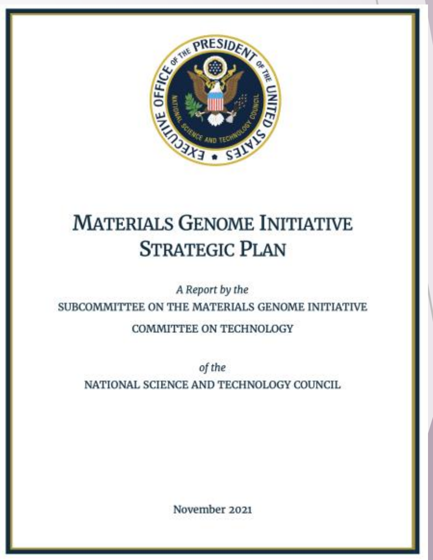
Exec Sec

J A Warren
NIST

Materials Development Continuum







MATERIALS GENOME INITIATIVE STRATEGIC PLAN

A Report by the

SUBCOMMITTEE ON THE MATERIALS GENOME INITIATIVE

COMMITTEE ON TECHNOLOGY

of the

NATIONAL SCIENCE AND TECHNOLOGY COUNCIL

November 2021

Traditional path is too slow
- Linear
- One-directional

Accelerated path
- Multifaceted
- Iterative

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MGI Strategic Plan 2021 (MGI 2.0)

1. Unify the materials innovation infrastructure
2. Harness the power of materials data
3. Educate, train, and connect the materials R&D workforce

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MGI is a culture shift

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MGI Goal 1: Unify the Materials Innovation Infrastructure (MII)

Bridge, Build, and Bolster the elements of the MII

Data Infrastructure

Experiments

Synthesis/Processing
Structure
Properties
Performance

Computation

Integrated research platforms

Foster a National Materials Data Network

Data Generators

Product Development
Manufacturing
Reuse/Recycling

Data Users

Accelerate adoption of the MII through National Grand Challenges

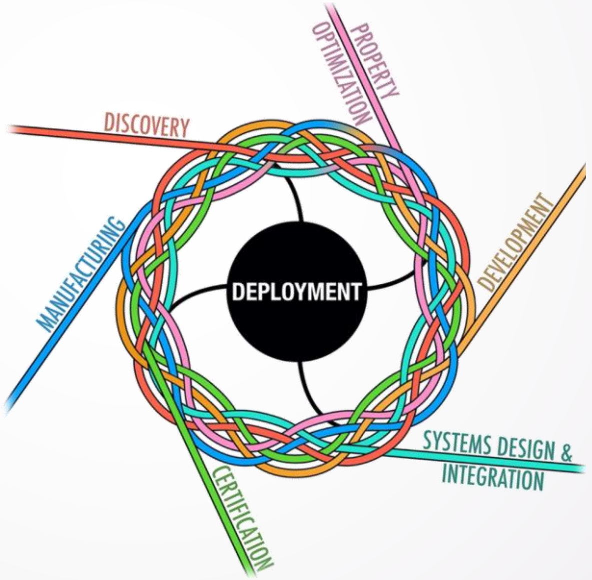
2018 NIST-Commissioned Report[1]
US benefit of an improved MII
$123 B/yr to $270 B/yr

[1]See: https://www.nist.gov/mgi

MGI Goal 2: Harness the Power of Materials Data

Accelerate materials R&D deployment through application of artificial intelligence (AI)

AI driven
synthesis/processing
structure
properties
performance
systems-based integration



MGI Goal 3: Educate, Train, Connect the Materials R&D Workforce

Objective 1:
Address current challenges in materials R&D education

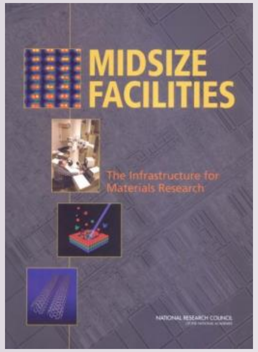
Objective 2:
Train the next-generation workforce

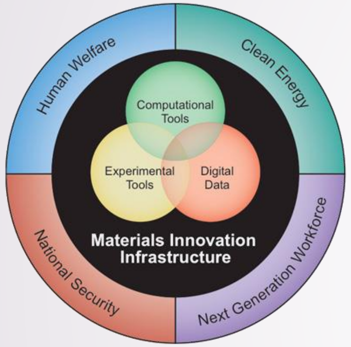
Objective 3:
Connect talent to opportunity

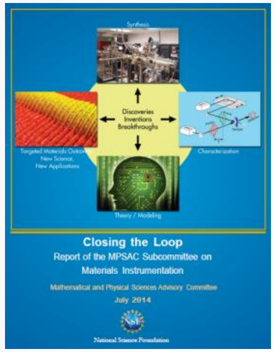
www.tms.org/MGIWorkforce

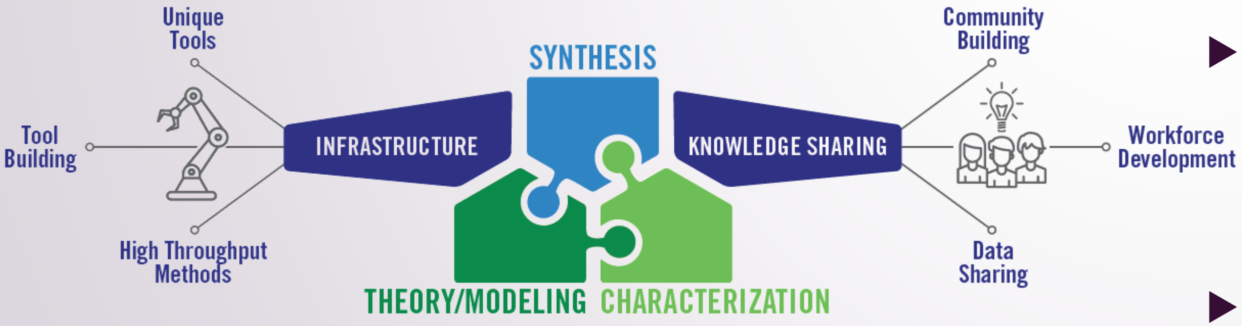
MATERIALS INNOVATION PLATFORMS

Materials Innovation Platforms (MIP)





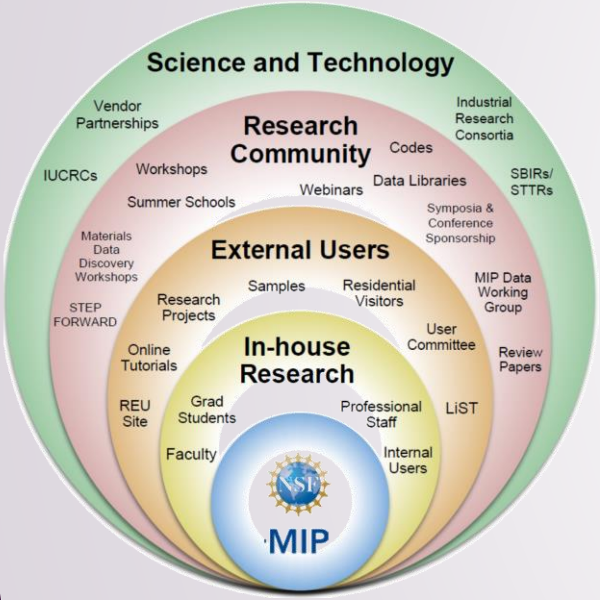




- A relatively new mid-scale infra-structure program in DMR: two competitions in 2015 and 2019
- Uses the Materials Genome Initiative (MGI) approach
- Designed to accelerate advances in materials research topics of national importance
- Builds and nurtures a scientific ecosystem through knowledge sharing (instruments, codes, samples, data, metadata, know-how, ...)
- Instrumentation & Technique development

PARADIM
2D Crystal Consortium NSF Materials Innovation Platform
BioPACIFIC Materials Innovation Platform
GlycoMIP

4 Pillars of MIP Convergence



1. Use an integrated approach to meet the critical needs for research, education/training, and research infrastructure

2. Foster a culture of knowledge sharing among in-house research scientists, external users, and other scientists

3. Enable iterative, closed-loop efforts across materials synthesis/processing, materials characterization, and theory/modeling/simulation

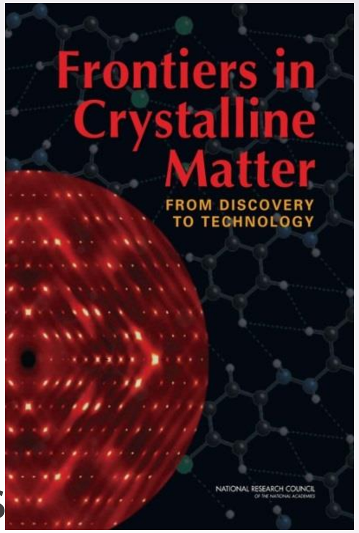
4. Empower the merging of ideas, approaches, and technologies from widely diverse fields of knowledge (domain science fields relevant to MIP, data science, informatics, ...)

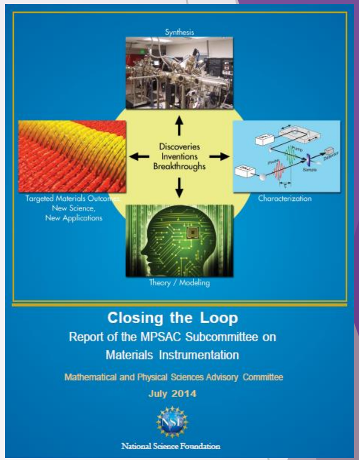
What Does a MIP Do?

- **Develop** next-generation experimental and computational **tools**, as well as advancing the capabilities of the current state-of-the-art tools
- Conduct **in-house research** by a transdisciplinary team in a focused topic designed to address a grand challenge of fundamental science and meet a national need
- Operate a **user facility** that provides unique materials research tools, samples, data, and technical services open to a diverse community of external researchers and institutions
- Serve as an educational focal point for **training** the next generation of tool developers and users

In this manner, a MIP will build and nurture **a scientific ecosystem**, which includes in-house research scientists, external users and other scientists who share tools, codes, samples, data, and know-how in order to strengthen collaboration among the scientists and enable them to work together in a new modality.

The First MIP Competition





- When: 2015
- Topic: Bulk and thin-film crystalline hard materials
- Statistics:
  - 4 finalists invited to reverse site visit at NSF in August 2015
  - 2 awards made in March 2016 (5 years, plus a 5-year renewal based on performance. 10 years maximum)
    - ✓ **PARADIM and 2DCC**
- Both 2016 MIPs successfully renewed in 2021

PARADIM
AN NSF MATERIALS INNOVATION PLATFORM

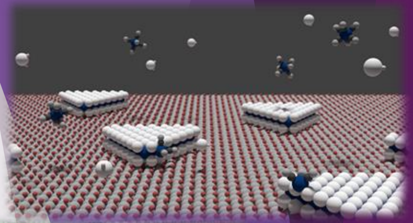
2D Crystal Consortium
NSF Materials Innovation Platform

2D Crystal Consortium

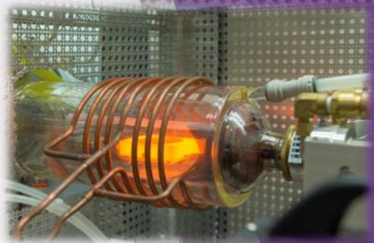
NSF Materials Innovation Platform

www.mip.psu.edu

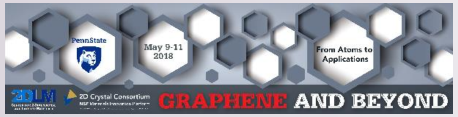
PennState



- Focus: Layered chalcogenide crystals and related 2D materials
- Major User Facilities (all at Penn State University):
  - Thin-film growth: CVD, MBE with STM, SEM & laser ARPES (new) in HIVE, and confinement heteroepitaxy (upcoming)
  - Bulk crystal growth: Bridgman & chemical vapor transport furnaces
  - Theory and simulation: growth kinetics, characterization, *etc*.



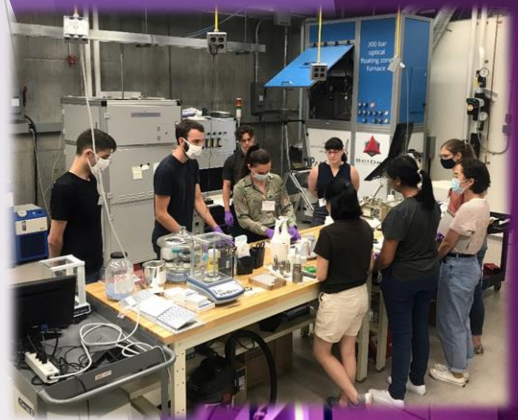
- Major Activities:
  - Accept user proposals year round
  - Sample, data, and ReaxFF request options
  - Annual *Graphene and Beyond* workshops
  - Webinars (all recorded and available online)
  - Resident Scholar Visitor Program
  - Data: Lifetime Sample Tracking (LiST) and LiST 2.0 (artificial intelligence), STEPFORWARD



PARADIM

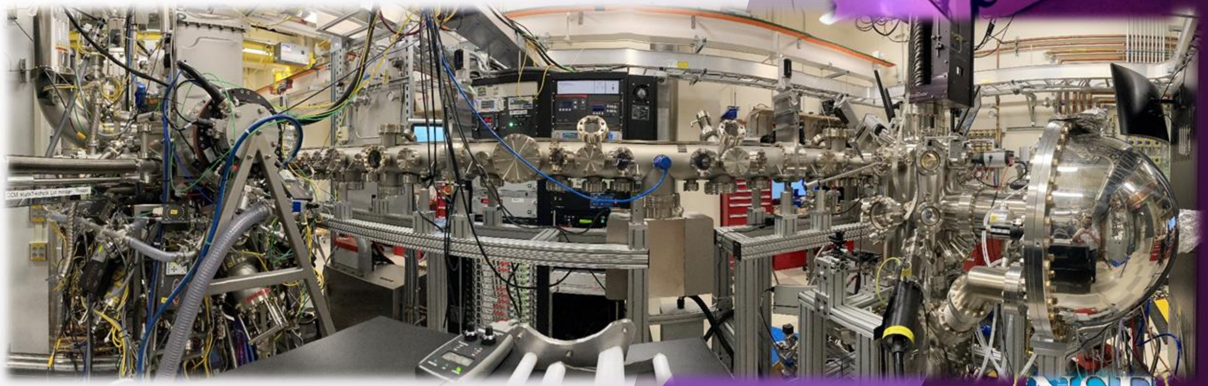
AN NSF MATERIALS INNOVATION PLATFORM

www.paradim.org

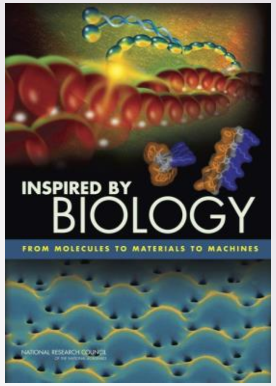


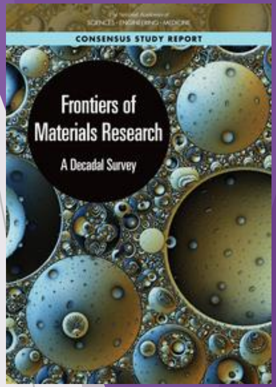
- Focus: Inorganic single crystals and epitaxial thin films with superior electronic characteristics, particularly interface quantum materials
- Major User Facilities (at Cornell University unless otherwise noted):
  - Thin-film growth: MBE (62 elements) with ARPES & laser sample heating (upcoming)
  - Transmission Electron Microscopy (Spectra) with 2nd-generation EMPAD (new)
  - Theory and Simulation: electronic properties and mismatched interface theory
  - Bulk crystal growth (at Johns Hopkins): world's first floating-zone furnace (FZF) with 300-atm O_2, tilted laser-diode FZF, and laser-heated 1000-atm pedestal furnace

- Major Activities:
  - Accept user proposals year-round
  - Summer schools (all recorded & available online)
  - Public data sets and analysis codes associated with published papers available at PARADIM website (new)

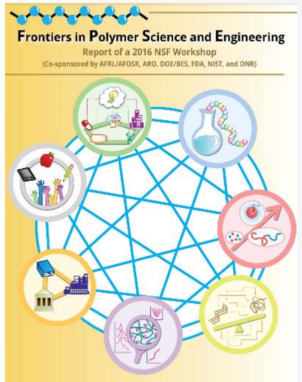


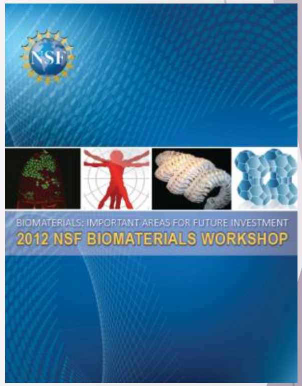
The second MIP Competition

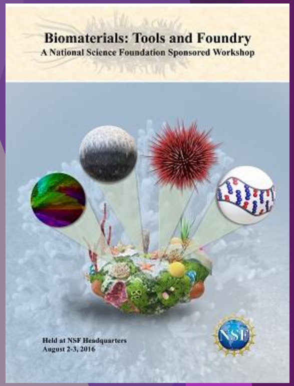




- When: 2019
- Topic: the convergence of materials research with biological sciences for developing new materials
- Statistics:
  - 4 finalists invited to reverse site visit at NSF in November 2019
  - 2 awards made in August 2020 (5 years, plus a 5-year renewal based on performance. 10 years maximum)
    - ✓ BioPACIFIC MIP and GlycoMIP







BioPACIFIC
NSF Materials Innovation Platform DMR-1933487

GlycoMIP
AN NSF MATERIALS INNOVATION PLATFORM

BioPACIFIC

NSF Materials Innovation Platform DMR-1933487

NSF

www.biopacificmip.org

UCSB UCLA

- Focus: Scalable production of bio-derived building blocks and polymers from yeast, fungi and bacteria. Data-driven discovery of next-generation polymers with properties and performance far exceeding those currently available in materials produced through traditional petrochemical-based methods.
- Major User Facilities: (at UC Santa Barbara and UC Los Angeles):
  - Living Bioreactor: automated gene assembly, amplification, transformation, strain growth, and metabolite analysis (UCLA)
  - Synthetic Chemistry: robotic synthesis, flow chemistry, and 3D printing (UCSB)
  - Characterization: Next-generation XRD, microRheology (UCSB); microED (UCLA)
  - Data and Computation: multiscale biopolymer simulation (UCSB)

- Major Activities:
  - Accept user proposals & sample requests year round
  - Summer schools on industry workforce development
  - BioPACIFIC MIP *Monomer* and *Pathways Libraries*

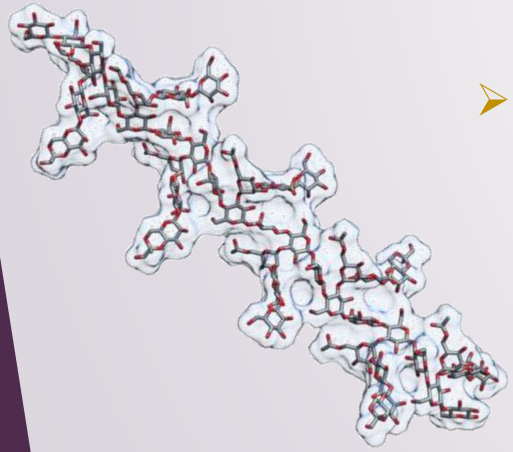
GlycoMIP

NSF Materials Innovation Platform

www.glycomip.org

VIRGINIA TECH · UNIVERSITY OF GEORGIA · Brandeis UNIVERSITY · Rensselaer · THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL

- **Focus:** Rational design and development of novel glycomaterials
- Major User Facilities (at Virginia Tech and the University of Georgia):
  - On-demand glycan synthesis: two automated glycan synthesizers
  - *De novo* structure determination: expert services on state-of-the-art spectrometers
  - Biomolecular interaction analysis: high-throughput and automated instrumentation
  - Solution-state 3D structure analysis: Raman and infrared optical activity
  - Theory and simulation: virtual user facility for glycan modeling

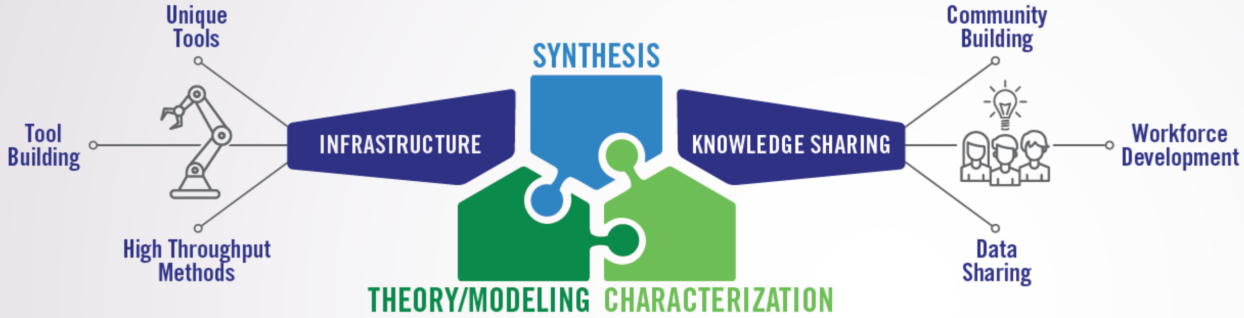


- Major Activities:
  - Year-round acceptance of proposals and sample requests
  - Summer schools and hands-on training courses
  - Open-access webinars and educational videos
  - Open-access databases (spectra, molecular models, synthesizer data)

MATERIALS INNOVATION PLATFORMS

Materials Innovation Platforms (MIP)


Charles Ying   Cosima Boswell-Koller



PARADIM · 2D Crystal Consortium NSF Materials Innovation Platform · BioPACIFIC Materials Innovation Platform · GlycoMIP

For more information, visit www.mip.org

Discussion

How do the MRSECs contribute to, strengthen, and bolster the Materials Innovation Infrastructure?

- Are there key initiatives already underway? If so, what are they?
- Are there current activities that could be leveraged and strengthened through collaborative efforts amongst many/all MRSECs?
- Are there activities the network of MRSECs or subsets of MRSECs could develop?

How can the MRSECs best communicate their collective impacts in support of the materials community?

Thank you

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