The Molecular Foundry at Berkeley Lab

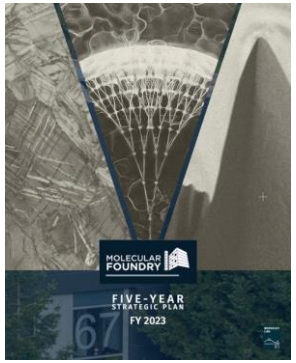
Positioned Within a Vibrant, Creative Scientific Ecosystem

- Adjacent to UC Berkeley and close proximity to Silicon Valley
- Co-located with other national user facilities, Energy Innovation Hubs, and Energy Frontier Centers at Berkeley Lab

Composed of 7 'technical facilities' driven by synergistic activities in synthesis, characterization, fabrication and theory

Guided by Five Cross-Cutting Research Themes Detailed in Our Five-Year Strategic Plan

- Architecting Information-Dense Multi-scale Materials
- Atomically Precise Control of Energy and Information Flow
- Nanoscale Science Towards a Sustainable Future
- Accelerated Materials Discovery and Prediction
- Physical and Digital Infrastructure as Drivers for Innovation



Served users from 36 countries and 622 institutions since opening.

BERKELEY LAB MOLECULAR FOUNDRY | Brookhaven National Laboratory Center for Functional Nanomaterials | Argonne NATIONAL LABORATORY Center for Nanoscale Materials

U.S. DEPARTMENT OF ENERGY | Office of Science

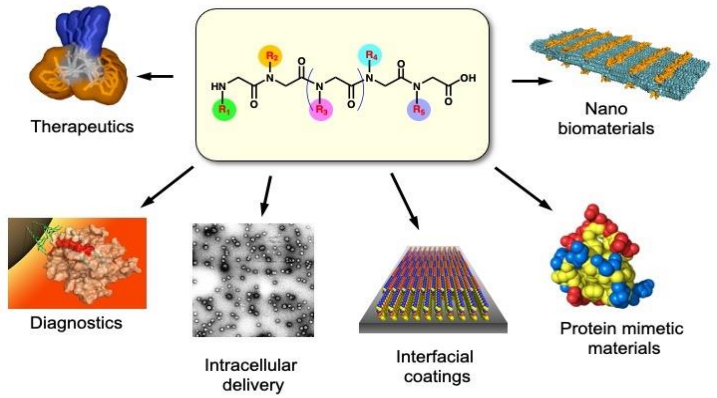
OAK RIDGE National Laboratory CENTER FOR NANOPHASE MATERIALS SCIENCES | Sandia National Laboratories | CNM | Los Alamos NATIONAL LABORATORY

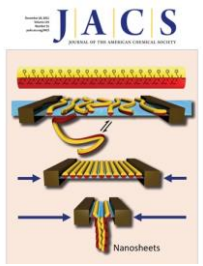
Scientific Leadership from the Molecular Foundry

Sequence-defined Hierarchical Peptoids

- **Peptoids:** novel, bio-inspired polymers capable of self-folding into protein-like structures.
- Synthesized by **robot-accelerated** workflows
- Antiviral agents, biomedical antifreeze molecules, detecting toxins, purifying water etc.

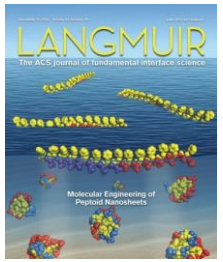
5 Peptoid companies launched through Foundry's user program
180 user projects and 150 publications
11th Annual Peptoid summit >220 participants





Zuckermann 2011

Zuckermann, Gang 2022



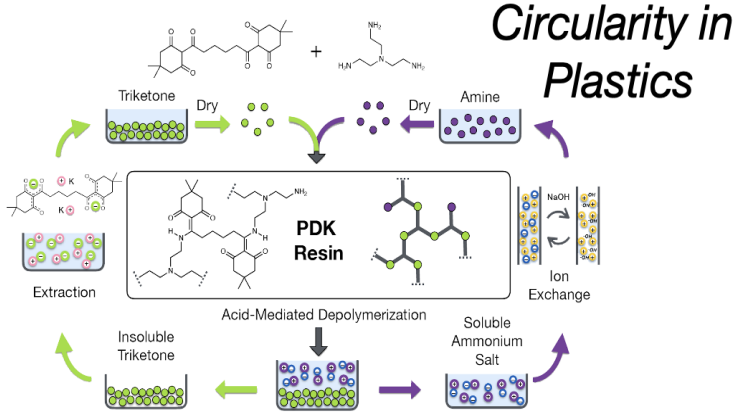
Connolly, Zuckermann, 2016

Fully Recyclable Polymers

- New family of **plastics** referred to as polydiketoenamines (PDK)
- **Deconstructed to their original monomers** in high yields and purity for full cyclic reuse.
- Collaboration with JBEI enabled engineered microorganisms to produce the **raw materials** used in PDK materials **from biorenewable sugars** such as corn stover.
- DOE ENERGY Icorps program → Cyklos Materials, to commercialize the technology as biorenewable **circular replacements for polyurethane**.

CYKLOS

MOLECULAR FOUNDRY | JBEI Joint BioEnergy Institute | The Materials Project



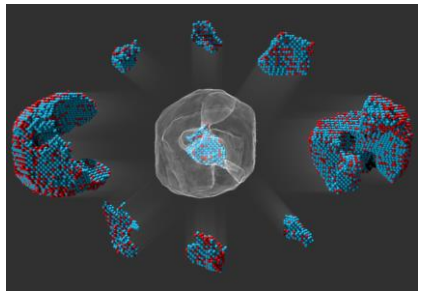
Helms Sci. Adv. **2022,** *Science* **2021**, *Nat. Chem.* **2019**

Pioneers in advanced electron microscopy

- Pioneer in **technique and instrumentation development** for nanoscale characterization with **electrons**.
- Extended atomic resolution microscopy to 3D.
- Led developments in electron detector technology and **large-data analysis** that enabled 4D nanodiffraction imaging for unprecedented **multimodal** nanoscale quantification.

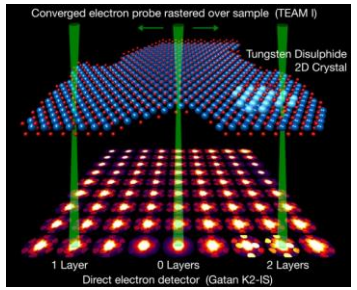
Over 1500 publications in electron microscopy
Multiple unique Foundry-developed platforms
Analysis code downloaded >100,000 times

from 2D to 3D

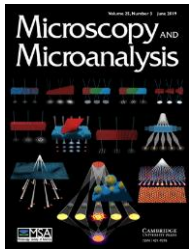


Identification of all 23,000 atoms in a nanoparticle with 20 pm 3D precision

…to 4D



LBL-developed 87,000 Hz electron detector for 4D-STEM



Ophus 2019

Ercius 2020

Minor 2021

Molecular Foundry Synergy with other User Facilities

20% of users engage ALS

16% of users engage NERSC

Users increasingly engage Materials Project

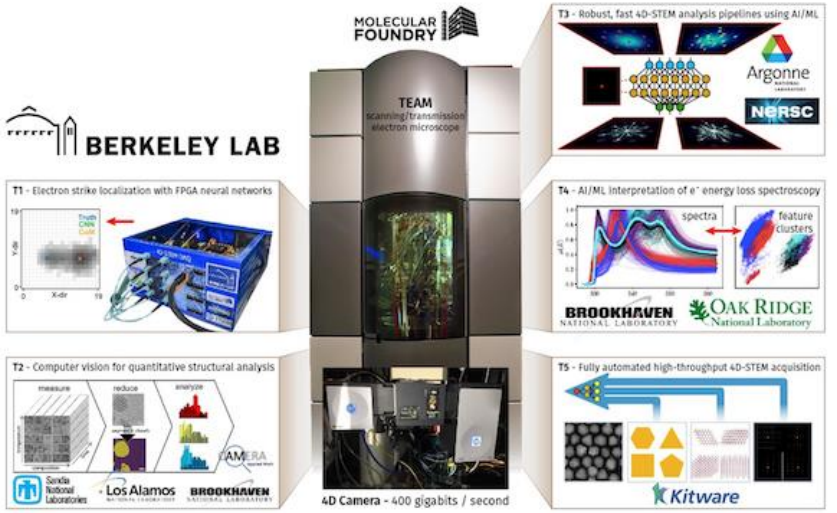
Berkeley Lab Co-location advantage:

- **NERSC:** Data pipelines to for real-time HPC analysis
- **ALS:**
  - Shared data infrastructure on correlated experiments
  - Autonomous Synthesis pipelines connect to in-situ characterization
- **Joint Genome Institute:** Co-appointed Staff Scientist
- **Advanced Quantum Testbed for QuBit circuit characterization**
- **Materials Project** (co-PI Sinead Griffin, data group synergy)
- **CXRO:** State of the art high Numerical Aperture EUV-patterning tool

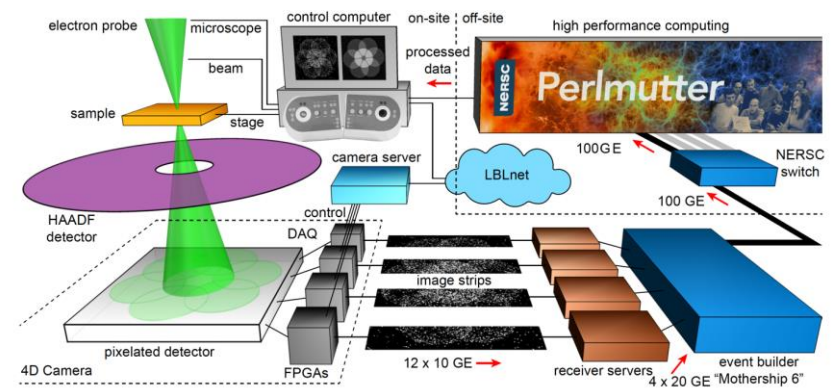
Software and Data Across the Complex

- Open-source tools shared across NSRCs and Light sources
- 4D Camera Distillery: All-NSRC + NERSC collaboration to process and visualize high rate (7 TB/min) data acquisition and develop ML tools
- MLExchange: Collaboration between light-sources,Foundry, CNM, and CNMS to create a user accessible ML analysis pipelines

4D Distillery: Foundry-led All-NSRC collaboration for ML pipelines in EM



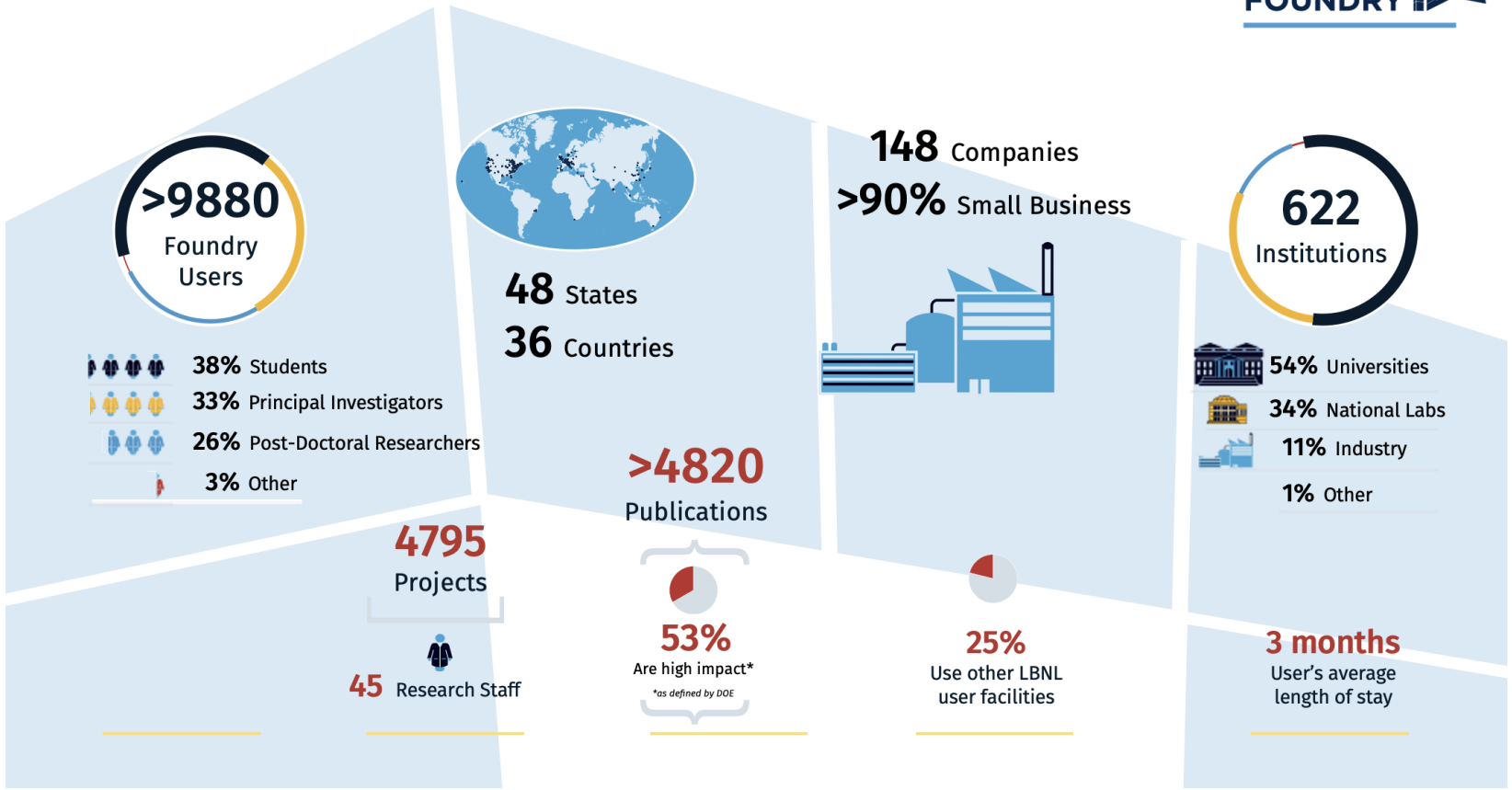
Direct connection of 100 gbps detectors to NERSC for on-stream processing

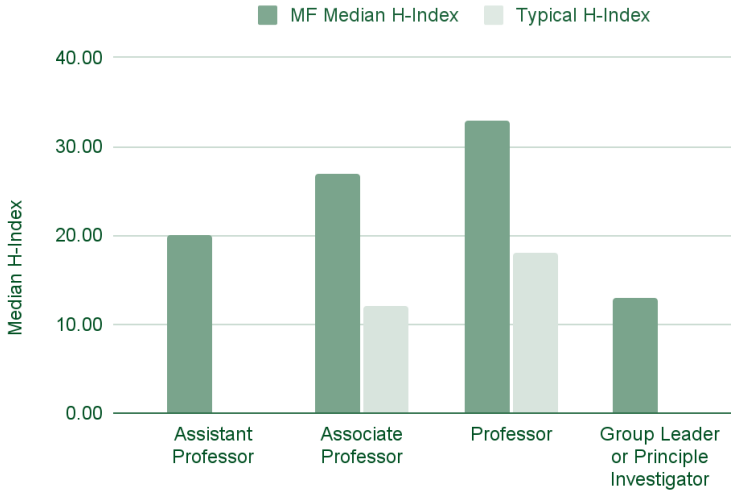


Molecular Foundry User Program

SMALL SCIENCE. BIG IMPACT.

MOLECULAR FOUNDRY





Workforce Development

Foundry postdoc alums have 2x median h-index in their future careers

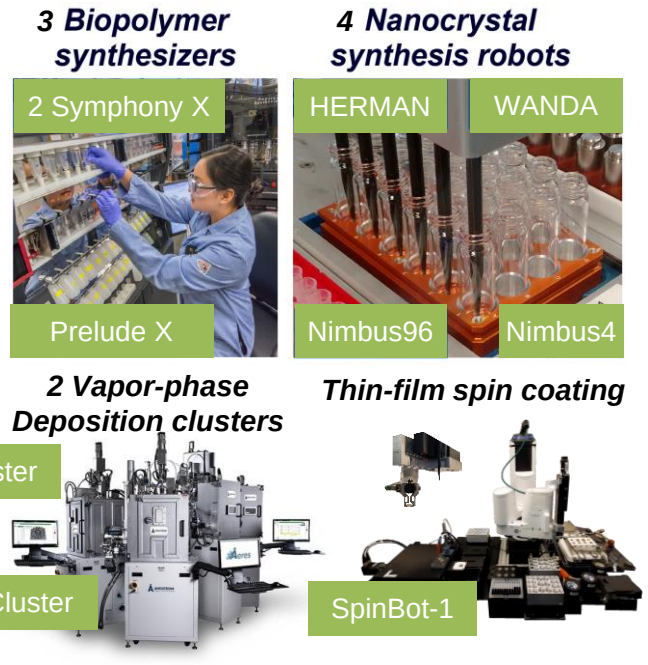
Outreach Efforts

- Proposal Acceptance rate parity across gender and MSI/R1 institutions
- Plan to add MSI Outreach staff under Optimum Operations
- User outreach at Diversity-centered Conferences (SACNAS, NSBE, SWE)
- Active outreach to Current and Prospective Users about RENEW and FAIR opportunities
- MSI Personnel in Proposal Review Board, User Meeting, User Executive Committee

In FY22 alone: >950 Users, >400 Publications (54% with IF > 7), 25 Countries on 6 continents

Future Vision for the Molecular Foundry

10 Robot Assisted Workflows

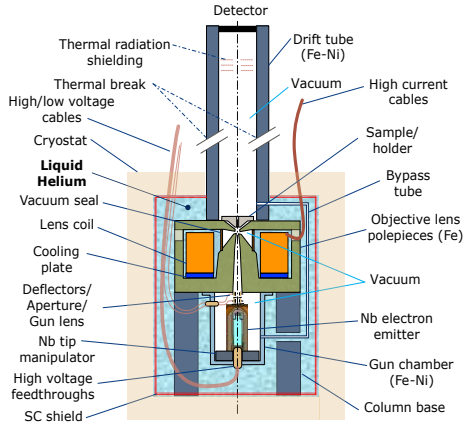


Accelerating Discovery

- Closed-loop AI-guided synthesis on 7 robotic platforms
- Push labeled synthesis data from automated experiments to Materials Project for open access and training of kinetically-aware models
- Integrated data pipelines with live analysis on NERSC
- Inverse design of complex heterostructures

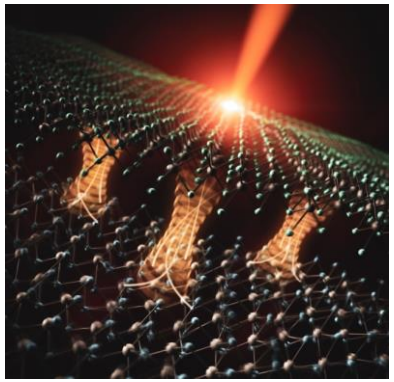
All-superconducting Electron Microscope (1K-TEM)

- Atomic resolution structure and spectroscopy of quantum materials to map quantum behavior
- Low-T behavior and coupled processes at interfaces
- Unmatched stability of lens currents, electron source, and sample stage



Quantum Information Science

- Atomic control 0D, 1D, and 2D heterostructures for understanding decoherence and quasiparticle engineering
- Autonomous synthesis of SC QuBit devices with atomic characterization and device screening
- Unique QSPLEEM: nanoscale magnetic imaging and spectroscopy with 3D spin resolution of quantum phases



The Biomaterials Genome Project

Tapping the undiscovered natural resources of genomes to discover the Next Generation of Biomaterials

New joint effort with the Joint Genome Institute

MOLECULAR FOUNDRY

JGI JOINT GENOME INSTITUTE