Five-Year Strategic Plan

FY 2018

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1. Executive Summary

The Molecular Foundry is a knowledge-based User Facility for nanoscale science at Lawrence Berkeley National Laboratory (LBNL), supported by the Department of Energy (DOE). As an integral part of the LBNL research community, the Foundry contributes strongly to each of the Lab's strategic initiatives focusing on Advanced Biogenics Chemicals and Materials, Machine Learning for Science, and the Water-Energy Nexus, as well as key priorities in Quantum Information Science (QIS) and Next-Generation Electron Microscopy.. The Foundry's mission is to provide communities of users worldwide with access to expert staff and leading-edge instrumentation to enable the understanding and control of matter at the nanoscale in a multidisciplinary, collaborative environment. Users come from academic, industrial and national laboratories, both domestic and international, at no cost for non-proprietary research. They gain access to the Foundry on the basis of a competitive external peer-reviewed proposal process.

The Molecular Foundry is producing a body of world-class, high-impact fundamental user research that is advancing the forefront of nanoscale science. This research portfolio not only maintains the center's leadership position in the world of nanoscience but also forms the foundation of scientific expertise that attracts the next generation of users to the Foundry. The Foundry's four multidisciplinary research themes focus the center's existing, leading-edge research in nanoscience and nanotechnology, its ambitious future, and strategic areas of opportunity for which the Foundry is best positioned to support and advance DOE's basic energy sciences mission.

This **Molecular Foundry Strategic Plan** focuses on the specific scientific drivers within these four themes that guide the Foundry's mission to share expertise with its expanding user communities in the next few years. Strategic future directions within each scientific theme, building on established strengths and leveraging our specific local environment at LBNL and throughout the Bay Area, are discussed in detail and summarized here:

- Combinatorial Nanoscience
    - Colloidal Nanocrystals
    - Molecular Folding Science
    - Framework Nanomaterials
- Functional Nanointerfaces
    - Dynamic Nanointerfaces: Directing Energy Flow and Chemical Transformations
    - Engineering Low-Dimensional Nanomaterials Across the Periodic Table
    - Functional 3D Hybrid Architectures from Designed Nanointerfaces
- Multimodal Nanoscale Imaging
    - Imaging Function and Interaction in Buried Environments
    - Mapping of Fields in Space and Time
- Single-Digit Nanofabrication and Assembly
    - Precision Two-Dimensional Patterning
    - Precision Three-Dimensional Nanofabrication
    - Controlling Function Through Precise Structures

This strategic plan describes routes to realizing the potential of the opportunities listed above. While it is not meant to be comprehensive, nor does it mention every research area or approach that will be pursued in the coming years, it is a broad scientific and organizational outline that will serve to guide the Molecular Foundry while enabling us to adapt to the rapidly changing research landscape.

2. Introduction

Supported by the Department of Energy Office of Basic Energy Sciences (BES) through their Nanoscale Science Research Center (NSRC) program, the Molecular Foundry is one of five national User Facilities for nanoscale science that serves nearly 1000 academic, industrial and government scientists around the world each year. Users come to the Foundry to perform multidisciplinary research beyond the reach of an individual's own laboratory. By taking advantage of the Foundry's broad spectrum of core capabilities and expertise, users increase the scope, technical depth, and impact of their research. Moreover, while at the Foundry, users access LBNL's diverse scientific community that includes other user facilities, including the Advanced Light Source (ALS) and National Energy Research Scientific Computing Center (NERSC), as well as the Energy Innovation Hubs, such as the Joint Center for Artificial Photosynthesis (JCAP) and Joint Center for Energy Storage Research (JCESR), Joint BioEnergy Institute (JBEI), and a number of local Energy Frontier Research Centers (EFRCs).

The Molecular Foundry features world-class scientists with expertise across a broad range of disciplines and state-of-the-art, often one-of-a-kind, instrumentation. Staff spend at least half their time working with outside users that are selected through an external, peer-review process. Staff then devote the remainder of their time to internal research activities, which can be augmented with postdoctoral fellows hired using internal or external grant support. Internal research programs advance the frontiers of nanoscale science by developing new capabilities that are made available to users. In this novel feedback model that was created by the Molecular Foundry and its fellow NSRCs, users are strongly engaged to advance Foundry research: many new Foundry capabilities arise out of synergistic projects with users.

Nanoscience can open new frontiers in energy, electronics, materials science, and biology. Research conducted with users at the Molecular Foundry defines these new frontiers and develops science and technology strategies to enable them. Organized into seven interdependent research facilities that support the four crosscutting scientific themes, the Foundry provides access to state-of-the-art instrumentation, unique scientific expertise, and specialized techniques to help users address myriad challenges in nanoscience and nanotechnology.

At the Molecular Foundry, a vibrant, growing, and increasingly engaged community of users combines with a well-recognized, highly-productive staff. At the start of FY18, the Foundry includes 24 independent researchers plus 3 active recruitments and 18 technical staff with 1 active recruitment. At the same time, while the Foundry features in-house state-of-the-art instrumentation, several capabilities are nearing the end of their lifecycle. Motivated by theeleven scientific future directions described below, this plan addresses these areas of need while also evolving the Foundry's scientific themes in step with the frontier of nanoscale science.

2.1 Foundry Research Facilities and Themes

The six-story, 94,000 square-foot Molecular Foundry building at LBNL overlooks the UC Berkeley campus and, from a distance, the San Francisco Bay. Directly adjacent to the Foundry is the

National Center for Electron Microscopy (NCEM) complex that was established in 1983 to maintain a forefront research center for electron microscopy of materials with state-of-the-art instrumentation and expertise. In 2014, NCEM merged with the Molecular Foundry to take advantage of growing scientific and organizational synergies. Each of the six floors of the Foundry building, as well as NCEM, is managed as a technically distinct "facility" by world-class scientists equipped with state-of-the-art instrumentation, laboratories, and computational resources.

Summary of the Seven Technical Facilities

Imaging and Manipulation of Nanostructures

This facility develops and provides access to state-of-the-art characterization and manipulation of nanostructured materials – from "hard" to very "soft" matter – including electron, optical, and scanning probe microscopies.

Nanofabrication Facility

This facility focuses on understanding and applying advanced lithographies, thin film deposition, and characterization, emphasizing integration of inorganic, organic, and biological nanosystems with the potential for nanoelectronic, nanophotonic, and energy applications.

Theory of Nanostructured Materials Facility

This facility expands our understanding of materials and phenomena at the nanoscale through development and application of theories and methods for excited-state and charge transport at nanoscale interfaces, self-assembly of nanostructures, and X-ray spectroscopy in complex nanostructured systems.

Inorganic Nanostructures Facility

This facility is devoted to the science of semiconductor, carbon and hybrid nanostructures—including design, synthesis, and combinatorial discovery of nanocrystals, nanowires, and nanotubes and their self-assembly into 3D mesoscale functional materials for use-inspired energy applications.

Biological Nanostructures Facility

This facility designs and synthesizes new materials based on the self-assembly of biopolymers and bio-inspired polymers, creates new nanocrystal probes for bioimaging, and develops synthetic biology techniques to re-engineer organisms and create hybrid biomolecules to interface with a variety of applications.

Organic and Macromolecular Synthesis Facility

This facility studies "soft" materials, including the synthesis of organic molecules, macromolecules, polymers and their assemblies, with access to functional systems, photoactive materials, organic-inorganic hybrid structures, and porous materials.

National Center for Electron Microscopy (NCEM)

A world-renowned center for microscopy since 1983, and integrated into the Molecular Foundry in 2014, this facility features cutting-edge instrumentation, techniques and expertise required for exceptionally high-resolution imaging and analytical characterization of a broad array of materials.

Four research themes

Four research themes at the forefront of nanoscience integrate users, staff and techniques across all seven technical facilities, embodying the Foundry's core capabilities and synergistic activities in synthesis, characterization, fabrication, and theory. They were reinforced through the strategic planning process described in Section 2.4 and are reviewed annually to evaluate their novelty, relevance, productivity, and impact. New capabilities and expertise developed in the context of internal research activities significantly augment the Foundry User Program.

Combinatorial Nanoscience

This theme focuses on the rational design of targeted nanostructured materials. Robotic synthesizers are used to generate large libraries of biological, organic, and inorganic nanostructures, which, in combination with theory and characterization, are used for discovery of new materials with sought-after optical, electronic and thermal properties.

Functional Nanointerfaces

This theme centers on understanding and design of the physical and chemical properties of hybrid nanomaterials, defined as integrated materials composed of highly contrasting components, such as inorganic nanomaterials, organic supramolecular assemblies, and complex living organisms. This is accomplished through the synthesis of heterostructures and interfaces, the application of first-principles simulations, and the detailed characterization of form and function.

Multimodal Nanoscale Imaging

This theme develops and applies multiple spectroscopic and imaging technologies – including high-resolution flagship electron microscopies, scanned probe microscopies, and hyperspectral (nano)optical methods and imaging probes – to investigate structural and dynamic nanoscale phenomena in hard and soft nanostructured materials in solid-state, liquid, and vapor environments. This theme takes on the characterization challenges associated with the continued development of novel and increasingly complex hybrid materials.

Single-Digit Nanofabrication and Assembly

This theme aims to organize and structure material with critical features of dimensions at or below 10 nm, i.e., on the single-digit nanometer and atomic scales, to create nanoscale devices and architectures in inorganic, biological, or hybrid systems. Work in this theme is accomplished by developing protocols to visualize, understand, and implement methods of self-assembly and lithography in a variety of systems.

2.2 User Program

As emphasized throughout this document, the Molecular Foundry User Program is central to our mission to provide the research community with access to an intellectual hub for multidisciplinary, collaborative research in a safe environment. By continually leveraging the new capabilities made possible by the Foundry's user and internal research programs, and also neighboring facilities including the ALS and NERSC, the User Program remains at the cutting edge of nanoscale science. An MOU allows users to jointly apply for time at the Foundry and ALS. Further synergies with the ALS, including a joint beamline and project scientist, are discussed in Section 3. At the same time, users of the Foundry also benefit from the annually allotted time provided by NERSC.

The Foundry's User Program is active and growing. In FY 2017, the Foundry received a total of 617 proposals (15% from industry) of which 77% were accepted and served a combined 866 onsite users (over 1000 total). These projects facilitate productive, high-caliber science: 355 publications, 33% of which were in high-impact journals as defined by the DOE. In addition, 40% of Foundry publications made use of one or more of the Foundry's co-located facilities at LBNL, most notably ALS and NERSC.

2.3 Vision for the Future

The Molecular Foundry's vision is to provide multidisciplinary communities of users the opportunity to develop, probe, understand, and control matter and its behavior at fundamental length scales to address the most important technological challenges in energy, the environment, and beyond.

To fulfill our mission, our broad institutional goals are to:

- Be a world-leading center of excellence for nanoscale science, producing and enabling impactful user-inspired research in innovative materials synthesis, advanced electron and optical characterization, and predictive theory and modeling
- Attract and foster strong collaborations with outstanding users from academia, industry and government laboratories worldwide. Provide all users with world-class facilities and a one-of-a-kind expertise, both at the Foundry and within the LBNL environment, working together to identify and address the biggest challenges in nanoscale science
- Play a central leadership role at LBNL and serve as a conduit for high-resolution imaging; organic, inorganic, and biological synthesis; nanofabrication and computational efforts
- Influence, educate and train the next generation of interdisciplinary scientists who will carry forward Foundry expertise, safety culture, and our inclusive and collaborative approach to research throughout their careers at other institutions and in industry

2.4 Planning Process

The Molecular Foundry Strategic Plan describes an ambitious agenda to guide the facility over the next several years. It is a living document that has been created in response to scientific and organizational needs of our users and staff, with input provided by the Foundry's Scientific Advisory Board (SAB) and a number of other outside stakeholders that represent the broad community of users.

As a DOE National User Facility, the Molecular Foundry's core mission is to provide world-class expertise and instrumentation that meet the needs of the greater scientific community. Accordingly, in summer 2014 a series of listening sessions with outside thought leaders – many of which are users – were organized by each of the seven facilities to solicit input on those areas where the Foundry can have the greatest impact. These discussions were centered on the following questions:

- What are scientific areas of particular promise/excitement/opportunity?
- What challenges must be overcome to take advantage of these opportunities?
- What are the most pressing needs that would help overcome these challenges? How could the Lab environment be leveraged toward these goals?

Initial listening sessions involved members of the Foundry's seven external Proposal Review Boards (PRB) that met with staff following their in-person proposal review meeting in May 2014. Later that month, additional meetings were held with local researchers from academia and industry in groups that corresponded to our seven facilities. Both sets of events with outside researchers representing the user community, along with input from internal meetings among staff, were used to create a list of nearly 100 scientific drivers in the area of nanoscale science and electron microscopy. This list was discussed and sorted into groups by Foundry staff. Though the process encouraged the potential creation of entirely new themes for the Foundry, in the end, this exercise reinforced that the existing scientific themes remained central to the interests of scientists outside the Foundry. It was also the genesis for specific future directions within each theme.

The contents of this version of the Molecular Foundry's strategic plan are the result of this deliberative process that included many diverse perspectives. In addition to the two sets of external listening sessions (who reviewed the final document following their initial input) and internal deliberations, the plan reflects the feedback of our SAB, the input of the scientific leadership of the ALS, and a number of other stakeholders, including the Foundry's User Executive Committee (UEC), who were also invited to contribute to the initial drafts. While these activities were initially motivated by the creation of this plan, an open channel of communication will be maintained with each of our constituents in order to continually meet the needs of our users.

The current Molecular Foundry's Strategic Plan builds off of the thorough planning activities of 2014. Since then, the plan has helped set priorities, guide leadership and inform the user community. Updates found in this new version reflect continuous dialogue with each of our many stakeholder groups, as well as planning activities such as the Foundry's annual Scientific Retreat, annual SAB Meeting , bi-annual PRB Meetings, monthly UEC Meetings, the DOE Operational Budget Review (February 2015), and the DOE Triennial Review (June 2016).

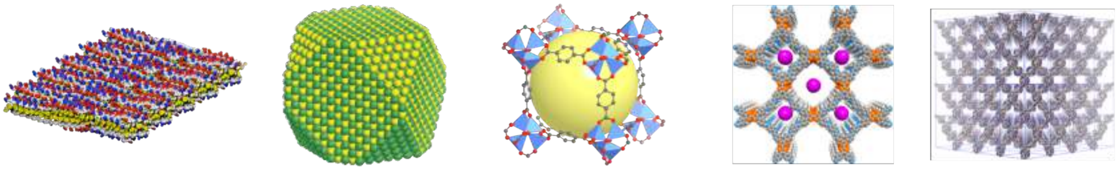
3. Plans to Leverage Emerging Scientific Opportunities

The introduction provided an overview of the Foundry and its vision as a knowledge-based DOE User Facility and premier research institution in multidisciplinary nanoscale science. In what follows, we describe specific scientific future directions within each of our four cross-disciplinary themes that best reflect the needs of the scientific user community and best capitalize on the Foundry's unique expertise and the scientific environment at Berkeley Lab. Each section also contains a number of planned capabilities – expertise and instrumentation – that are required to achieve the future directions of each theme, with essential participation from all seven scientific facilities.

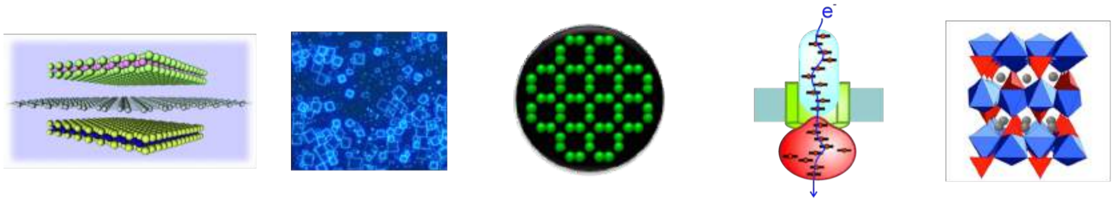
3.1 Combinatorial Nanoscience

Combinatorial Nanoscience at the Molecular Foundry embodies our interdisciplinary effort to develop capabilities for users to systematically design, synthesize, and characterize single-phase and hierarchical nanomaterials spanning several disciplines. Our singular focus on nanoscale materials is unique amongst contemporary combinatorial research efforts, as is our emphasis on using systematic, high-throughput exploration to extract novel scientific insight about the wide range of nanoscale phenomena of interest to our users and BES.

The Molecular Foundry will continue to invest broadly in capabilities to develop, synthesize, and understand a broad range of materials, including biomolecular assemblies, biomimetic polymers, inorganic nanocrystals, and organic and hybrid framework materials. New properties can emerge by tailoring not only their size and morphology, but also positioning chemically diverse atoms, domains, and functional groups at precise 3D locations within such materials. Nanostructured materials of this sophistication are to be programmed by multi-step chemical synthesis, where heterogeneous components are assembled in a particular order, each under specific conditions.



Protein-mimetic polymers **Inorganic nanocrystals** **Metal-organic frameworks** **Covalent organic frameworks** **Supramolecular organic frameworks**



2D materials (hybrid, TMDs) **Hybrid perovskites** **Mesoscale composites** **Biomolecular electron nanoconduits** **Battery materials**

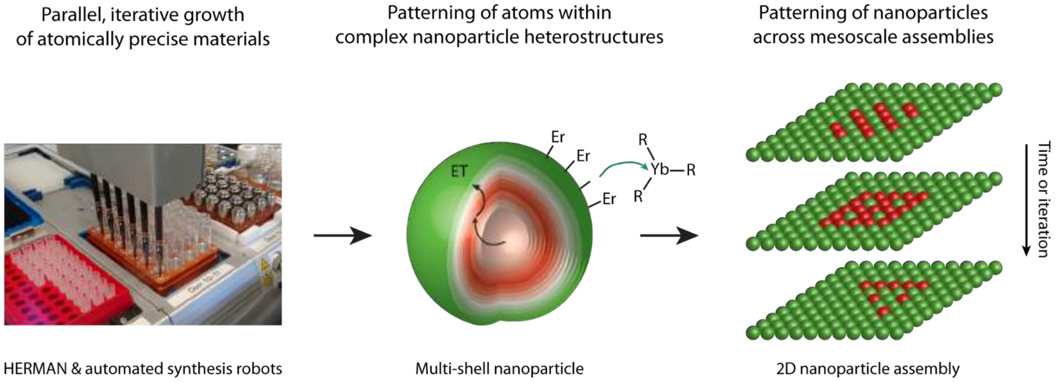
A diversity of nanomaterial discovery platforms under study at the Foundry.

Guided by the pioneering theoretical and chemical expertise of our staff, we will continue to establish automated synthesis workflows that focus on the reliable production of a diverse set of high-quality, precisely defined nanomaterials that serve a majority of our user and internal research projects. The insights and combinatorial tools strongly couple to, complement, and feed efforts in the Nanointerfaces, Multimodal Imaging, and Single Digit Nano themes to support a robust materials discovery platform.

Future Directions

Colloidal Nanocrystals

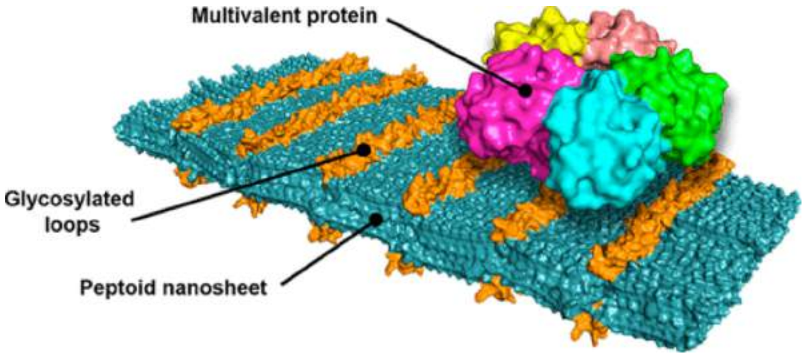
Across its facilities, the Foundry uses colloidal inorganic nanoparticles, small molecules and polymers, and in some cases living cells as modular building blocks to fabricate materials with mesoscale order that can store hydrogen, convert heat to electricity, sequester geologic CO_2 in minerals, and enhance efficiency of energy used in buildings. Precision control over the synthesis conditions enables the Foundry to provide the user community with reproducible nanoscale components, and it enables a fundamental understanding of their structure-function relationships. To create colloidal materials with ever-increasing complexity, we must be able to construct nanoparticles with atomic precision and high yield. We aim to achieve this using high-throughput robotic synthesizers that can iteratively grow atomic monolayers of inorganic and organic materials onto colloidal nanoparticles, allowing us to specify the elemental composition at exact points inside a nanoparticle. This capability will enable the design and fabrication of nanocrystal heterostructures that precisely control the position, flow, and energy of carriers, phonons, and dopant states. Such materials will be essential for extracting hot carriers in photovoltaic materials, controlling multi-excitonic processes in solid state lighting materials, and for manipulating complex energy transfer networks that give rise to non-linear optical processes. These deliberately synthesized building blocks will then be combined into mesoscale assemblies using analagous, particle-by-particle assembly methods. The well-defined, non-linear transport properties inside these heterogeneous assemblies may give rise to emergent phenomena, such as the nanoscale patterning of light, a process that could be analogous to the spontaneous patterning of organisms. Such mechansims align with BES Grand Challenges regarding biologically inspired materials and non-equilibrium matter. This research will harness the Foundry staff's considerable expertise in synthesis, assembly, characterization, and theory over multiple length scales, as well as those characterization capabilities of the ALS.



Atomically precise construction of complex nanocrystals and nanoparticle assemblies using 2nd generation high-throughput robotic synthesizers.

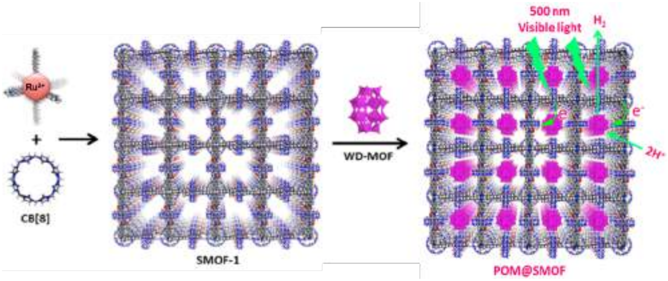
Molecular Folding Science

One of the BES grand challenges seeks to create technologies with capabilities that rival living things. We aim to do this by extending the architectural paradigm found in biology – the folding of linear, information-rich polymer chains into defined 3D structures – into the world of synthetic materials. We aim to become the premier Facility for the design, synthesis, purification, and engineering of sequence-defined polymers, characterizing and understanding their rules of folding and assembly, and creating nanostructured materials capable of complex, protein-like functions (e.g., molecular recognition and catalysis). Peptoid polymers are one of the most synthetically accessible family of sequence-defined materials known, whose synthesis by means of iterative covalent coupling reactions is so efficient and controlled, that we can now, for the first time, prepare high molecular weight polymers of defined sequence from a chemical diverse set of



Schematic of a glycosylated peptoid nanosheet binding a multi-valent protein.. [ACS Nano, DOI: 10.1021/acsnano.7b08018, (2018)] over 200 readily available monomers. Predictive multi-scale simulations will allow us to design new polymers that fold and self-assemble into well-defined nanostructures tailored to have ion channels, specific binding pockets, and efficient catalytic sites. Testing these predictions will require high-resolution structural characterization using cryoTEM, *in situ* AFM, and X-ray scattering at the ALS. Atomic-level structural characterization of these protein-mimetic nanoaterials will be possible with advances in electron microscopy that take advantage of spherical and chromatic aberration correctors, phase plate technologies, direct electron detectors for low-kV imaging, and the next generation of AFM probes for *in situ* imaging. The ability to both synthesize and characterize folded peptoid nanomaterials at the atomic scale will allow the precise engineering of their structures to optimize their function across a range of applications. This effort is expected to produce materials with the exquisite specificity of biological systems, yet also exhibiting the stability of traditional polymers. Such materials could be deployed in harsh environments to solve problems in separations, drug delivery, catalysis and sensing.

Framework Nanomaterials



Modular assembly of a 3D supramolecular metal-organic framework (SMOF) for use as a hybrid photocatalyst after incorporating catalytic POM anions into the framework via anion exchange [Nat. Commun., 7, 11580, (2016)]

Framework nanomaterials have attracted surging research interest for their open porous nanostructures, programmable surface features and tunable functionalities. The Molecular Foundry has established itself as a pioneer facility in metal-organic frameworks (MOFs), and has quickly expanded into the new framework materials space of covalent organic frameworks (COFs), supramolecular organic frameworks (SOFs) and supramolecular metal organic frameworks (SMOFs). While the extended family of framework materials enjoys functional complexity, the assembly scheme takes advantage of chemical interactions with different strengths and is quite modular. Combining our synthetic strengths with emerging capabilities in multi-scale simulation and high throughput characterization, we aim to explore an expedited approach to a broader range of framework nanomaterials with high structural and functional diversity. As manifested by the recent Theme Capability Development Program project entitled "A Combinatorial Approach to Multifunctional Porous Graphitic Materials (PGMs)" future efforts will be devoted to unite high-throughput synthesis, characterization, and multi-scale simulation to develop a robust materials discovery platform. Such efforts will open the door to a high-demand class of materials that have important energy applications in the areas of water desalination, CO_2 sequestration, energy storage, catalysis, and optoelectronics. TEM structure analysis at both nanoscale (high throughput) and atomic resolutions will provide critical feedback to the synthetic process by collecting structures and statistics of growth defects. *In situ* characterization under flowing gas environments will also provide information directly relevant to performance, and represents an entirely new capability for the Foundry.

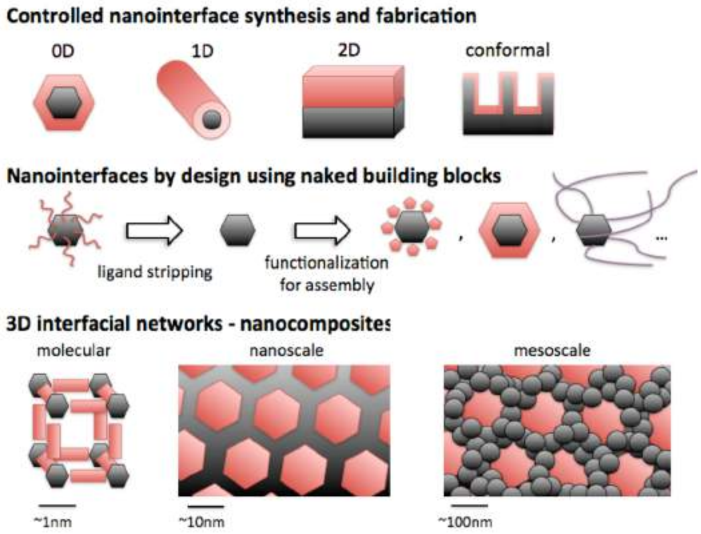
Planned Capabilities

High Pressure, High Temperature, Multi-Step Robotic Synthesizer

Our capabilities in high-throughput synthesis will be significantly enhanced by our next-generation nanocrystal synthesis robot—the High-throughput Experimentation Robot for Multiplexed Automation of Nanochemistry (HERMAN), early career staff scientists in the Inorganic Facility, and the recruitment of a new Organic Facility staff scientist. Using machine-learning algorithms closely integrated with theoretical models, the newly installed HERMAN will perform automated multi-step chemical synthesis at unprecedented temperatures and pressures. This will bring direct access to new classes of materials, such as complex nanocrystal heterostructures prepared through layer-by-layer growth and mesoscale architectures accessed through directed assembly. These new capabilities will complement those of WANDA, the first generation robot which remains a highly demanded tool, and the Hamilton Nimbus liquid handling robot, which enables the parallel synthesis of reactions in aqueous environments. This new robot will facilitate high-throughput screening of battery materials, conditions for nanoparticle bioconjugation, and porous framework materials synthesis and assembly.

Microfluidic Platforms for Parallel Synthesis and Characterization

As characterization techniques are developed that use ever smaller amounts of material, we aim to unite synthesis and screening on a single miniaturized device. Current investments in microfluidic infrastruture will lead to the creation of integrated microfluidic devices designed to facilitate real-time structural or functional feedback during the course of synthesis. This will accelerate nanomaterials discovery by enabling thousands of compounds to be prepared and screened in parallel. "Smart" synthesis chips will be developed that can evolve materials by *in situ* data analysis obtained by performing both parallel synthesis and screening steps. Nanomaterials discovered on these microscale devices will be validated by large-scale synthesis on the Foundry's robotic synthesizers.



The Molecular Foundry's synthesis and fabrication capabilities provide controlled approaches to create multidimensional interfaces spanning the nanoscale. Colloidal nanocrystals have insulating, inert coatings, which prevent easy coupling of nanocrystals for energy transfer. Naked nanocrystal building blocks can be assembled into molecular, nano- or mesoscale composites with nanoscale interfaces of controlled dimension and functionality

High-Throughput Characterization

In order to evaluate the structure and/or function of materials produced by our combinatorial synthesis engines with rapidity and efficiency, we will establish increasingly insightful high-throughput screening and characterization methods. We aim to establish automated electron microscopy methods, take advantage of robotic X-ray scattering and diffraction workflows at the ALS, and pursue electrochemical and spectroscopic approaches capable of evaluating hundreds of samples with minimal human intervention post-synthesis. Furthermore, we will benefit from close connections with applied mathematicians at LBNL through the new Center for Applied Mathematics for Energy Research Applications (CAMERA) to help build screening methods and bring tools of computational geometry, optimization, and machine learning.

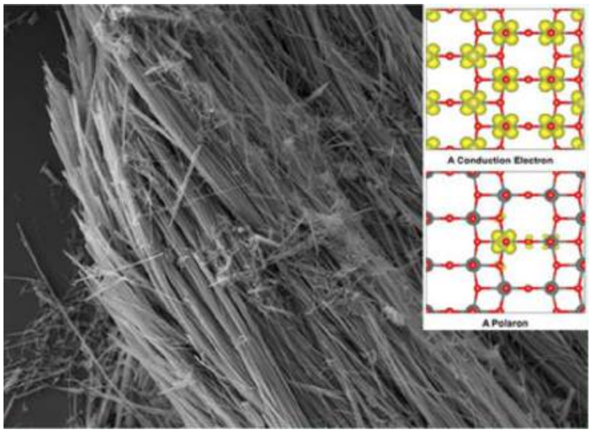
3.2 Functional Nanointerfaces

A frontier of materials science, and an area of increasing user interest, is the controlled integration of diverse nanoscale building blocks – e.g., inorganic, organic, biological – into functional mesoscale assemblies. As nanostructured building blocks intrinsically possess large surface-to-volume ratios, their assemblies feature a high-density network of nanoscale interfaces that present exciting new opportunities to control the propoagation of energy in hybrid materials. Spanning a diverse range of materials, the Functional Nanointerfaces theme at the Molecular Foundry drives the development of new capabilities for understanding and controlling both the sub-nanometer structure of individual interfaces and the mesoscale morphology of assemblies of interfaces. This effort aims to harness their unique characteristics both individually and collectively, for emergent functionality, particularly for quantum information science, energy conversion, storage, and conservation.

Interfaces can actively amplify or hinder the motion of charges, vibrational energy, light, or chemical information due to sharp contrasts in bonding modes, electronic energy levels and densities of states. There remains much to be learned about the exact nature of these emerging structural, electronic and dynamic properties and how they feed back across multiple length scales. However, a rich set of interdisciplinary scientific problems involve active transport processes at organic/inorganic, bio/inorganic, solid/electrolyte, and gas/solid interfaces. This theme involves cross-cutting activities spanning the creation of bottom-up 3D functional mesoscale assemblies with precisely controlled interfaces; development of new theoretical frameworks and computational tools for understanding and predicting static and dynamic properties of these interfaces; mapping of chemical transformations and energy flow across scales using advanced electron microscopy and the ALS; synthesis of macroscopic scale 2D transition metal dichalcogenides and engineering of their local electronic structure via atomic-level engineering of strain, defects, and heterojunctions; mapping optoelectronic and excitonic processes in 2D material-based structures at their native length scales; and detailed imaging and transport studies at these complex, buried, and dynamic interfaces.

Future Directions

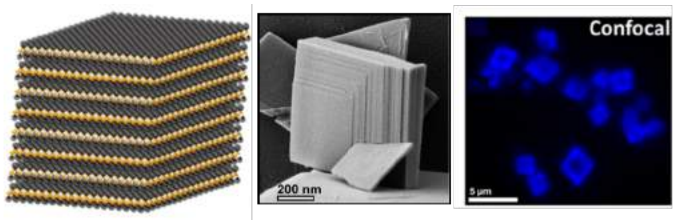
Dynamic Nanointerfaces: Directing Energy Flow and Chemical Transformations



Interactions between electrons and ions can slow down the performance of electrodes made with vanadium pentoxide. [Nat. Com., 7, 12022 (2016)]

Many renewable energy technologies depend critically on the efficient and reliable directional flow of charged (electrons, ions) or neutral (phonons, excitons, spin) excitations at interfaces. Additionally, chemical transformations across nanointerfaces are important for both the synthesis, nanopatterning, and function of many nanoscale materials with promising catalytic and energy storage applications. Over the next few years, we will advance our ability to chemically introduce orthogonal surface chemistries on arbitrary materials classes to enable new heteromaterial couplings. We will also advance *in situ* imaging capabilities for both hard and soft matter at various length scales and in relevant sample environments, while utilizing AFM and new approaches in advanced electron microscopy and scattering, as well as leveraging the ALS. Further, we will develop novel means to probe functional assemblies at the level of their nanoscale interfaces using microscopy, scattering, and spectroscopy to probe and validate interfacial structure under bias and illumination (described in Multimodal Nanoscale Imaging), as well as multi-scale theoretical models – from electronic structure to statistical mechanics – to guide and test hypotheses relating energy transport and chemical dynamics to changes in the size, composition, physical, or biological properties of constituent building blocks. We plan to tailor these capabilities for exploring novel functionality in environments that are out of equilibrium – e.g., conditions found in a battery, in a membrane, in a flow cell, or in a solar cell — and make them available to User communities both at the Foundry and the ALS.

Engineering Low-Dimensional Nanomaterials Across the Periodic Table



2D hybrid chalcogenides can be assembled in a 3D supramolecular crystal. Organic ligands serve to insulate inorganic layers from one another physically and electronically, enabling every layer to serve as an isolated, photoluminescent 2D material.

Metal chalcogenides are a broad material class of considerable interest for their diverse electronic, optical, mechanical, and catalytic properties. Examples include high-mobility semiconductors, superionics, high-Tc superconductors and topological insulators. The Molecular Foundry aims to develop a category of hybrid chalcogenide. Chemical design in hybrid materials affords an opportunity to build compounds in which the structure of a supramolecular lattice is intrinsically related to the function of the inorganic scaffold. Crystal engineering in the context of this approach will yield the capability to design and to engineer the band structure of semiconducting materials with atomic-precision. The central challenge is disentangling the complex structure-function relationships governed by metal coordination, ligand shape, and composition. A collaborative effort between several facilities at the Molecular Foundry and beamline 11.3.1 at the ALS will design, construct, characterize and redesign metal-organic chalcogenide nanomaterials over a broad composition range.

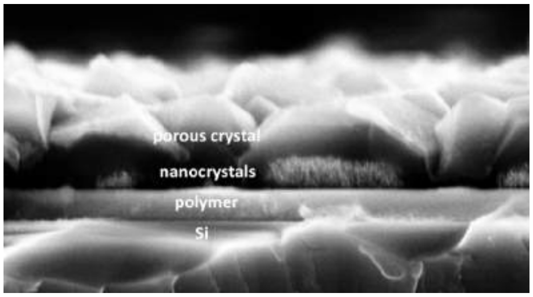
Joint Molecular Foundry-ALS Small- and Wide-Angle Scattering Beamline

Over the last few years, the Molecular Foundry has partnered with the ALS to develop high-throughput infrastructure (robotics and flight tube) on an ALSbeamline with advanced high-flux SAXS/WAXS capabilities for determination of nanoscale and mesoscale structure of soft and hybrid nano- and meso-structured materials. Operated jointly, the beamline enables broad and rapid access to Foundry users in need of this essential characterization tool for complex hybrid materials. This partnership will continue to facilitate research that takes advantage of both user facilities at Berkeley Lab and serves as a model for co-investments in interfacial science in the future.

Understanding how nature exploits electron-transfer in protein complexes provides new approaches to harness metabolism to drive electrons and energy across interfaces and into engineered materials.

Functional 3D Hybrid Architectures from Designed Nanointerfaces

The Foundry commands a diverse library of building blocks (as elaborated in the Combinatorial Nanoscience theme) that includes organic small molecules and inorganic clusters, synthetic and biological polymers, porous crystals, colloidal nanocrystals, 2D atomic layers (graphene, transition metal dichalcogenides, etc.), and even living cells. We have also begun to realize complex material hierarchies from these simple building blocks. We will develop approaches to place high quality 2D semiconductor materials on arbitrary substrates, creating local quantum wells, wires, and stacks of deterministic heterojunctions. Such unprecedented control over this material class will provide access to new quantum confined properties and the ability to incorporate this material class into devices. In the next 5 years, we will focus on elucidating the design rules by which desired functionality can be generated by exerting precise control over how individual components of arbitrary shape, size, and composition are assembled and ultimately interfaced. Given that assembly of matter emerges from a variety of driving forces during processing, understanding the energy landscapes and kinetics guiding both equilibrium and non-equilibrium assembly will be vital, and allow for more reproducible,



Controlling local chemical transformations at nanointerfaces yields complex heteromaterial architectures of porous crystals, colloidal nanocrystals, and functional polymers.

phase-pure materials to be generated. Success will require strategic investment in the development of both expertise and instrumentation to control and observe the evolution of structure across multiple length scales for a range of processing strategies on substrates with user-defined surface chemistry and topography, and as guided by the interfacial interactions between nanocomponents. We will develop capabilities that link, for the first time, computational simulations at the Foundry of mesostructured systems and their dynamics with time- and length scale-dependent X-ray scattering at the ALS and real-space evaluation of 2D and 3D structure and its evolution using *in situ* cells and electron tomography capabilities.

Planned Capabilities

Transition Metal Dichalcogenide Hetero-Junction Based Optoelectronic Devices

Ultrathin materials have attracted intense interest in the user community for photonic applications, but preparation of transition metal dichalcogenide (TMD) monolayer materials for applications is challenging. In partnership with the ARPES beamline at ALS, the Molecular Foundry is investing in bringing new synthetic capabilities for the preparation of wafer-scale, ultrathin materials by converting precisely deposited metal oxides directly into cutting edge materials, enabling a straightforward route to new technology based on TMD compounds and their heterostructures.

in situ Combinatorial Electrochemical Interface Imaging and Analysis Endstation

We will develop a suite of coupled *in situ* tools capable of probing both structure and transport at individual solid/electrolyte interfaces, and across statistical ensembles of interfaces, in reactive environments. This endstation will provide a window into electrochemical dynamics impossible to probe by the standard tools of electrochemistry. Understanding how interfaces influence chemical confinement, concentration fluctuations, and transport across these complex interfaces will serve crucial needs demanded by our global network of users, and also other local synergistic DOE investments such as the Materials Genome Initiative, Joint Center for Artificial Photosynthesis (JCAP) and Joint Center for Energy Storage Research (JCESR).

Engineering the transport of Energy across Biological Interfaces

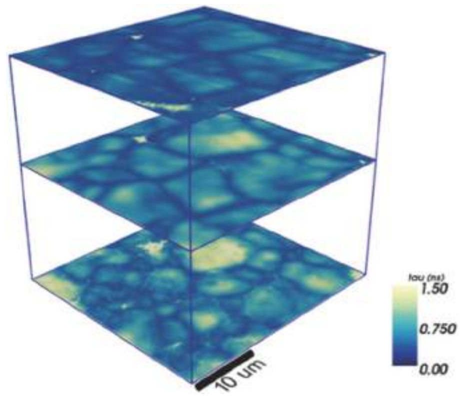
Microscale bacterial organisms have evolved a rich variety of strategies for exploiting energy from dilute sources in their environment, from sulfur-rich deep-sea volcanic vents to the dilute sources trapped inside glaciers. We aim to understand how organisms have evolved energy transport structures that enable them to shift electrons directly to and from a solid support on which they live. Understanding how organisms build a structurally complex buried protein-material interface that is inaccessible to traditional structural analysis is an area of intense interest by the Molecular Foundry and is an ideal target for collaboration with scientists at ALS. Understanding the biochemistry and physics of these evolved capabilities presents new opportunities to harvest energy directly from dilute sources using bacteria as a living electrical generator.

Mesoscale Theory for Functional Nanointerfaces from Electrons to Assemblies

Our aim of understanding materials and phenomena from the scale of electrons to assemblies requires us to tackle head-on the mesoscale challenge that is the coupling of distinct physical mechanisms across a broad range of length and time scales. To do so we will bridge our current many-scale theoretical capabilities in electronic structure and statistical mechanics – employing state-of-the-art mid-range cluster computing and enhanced by the current recruitment of a new staff scientist in our Theory of Nanostructured Materials facility – towards an integrated predictive multi-scale simulation framework. We aim, for example, to discover new materials made by the self-assembly of molecules at surfaces, using coarse-grained dynamical simulations whose force-fields are systematically parameterized using quantum mechanical calculations.

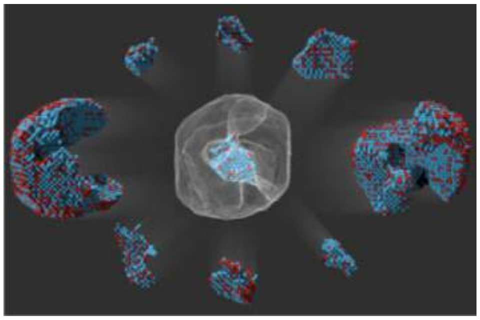
3.3 Multimodal Nanoscale Imaging

We are at the brink of a new era, where nanoscale building blocks can be assembled into complex heterogeneous materials, leading to architectures with entirely new physical properties capable of unprecedented functionality. While this capability offers extraordinary opportunities, it also presents a significant challenge: capturing, visualizing, and understanding the relationships between fundamental properties such as composition, material phase and atomic (dis)order, morphology, and electronic structure, and linking these to the resulting functionality within complex material systems. Imaging and correlating structure with properties and mechanisms at meso- and nanoscopic length, time, and energy scales under operating conditions is both an enabling capability and grand challenge for nanoscale science. This has been emphasized most recently by the DOE BES Report Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science, and the 2014 DOE BES report on the Future of Electron Scattering.



Two-photon tomography, a new method to map thin-film solar cells in 3-D [Adv. Mat., 29, 1603801 (2017)]

Multimodal Nanoscale Imaging is thus one of the four unifying scientific themes of the Molecular Foundry: multimodal, because we combine high-resolution electron scattering, local/scanning probes, multifunctional nanoscale reporters and time-resolved optical methods for studying both device-like and biological systems; and nanoscale, because we must understand material properties and processes at their native length scales, 10-100 nm. This theme investigates nanoscale systems in complex cellular, solid-state, liquid or gaseous environments, increasingly in relevant working conditions – for example, under bias, strain or illumination – and thus has focused on development of new technologies for *in situ* techniques. Our goal is to explore the basic principles underlying functionality by correlating chemical composition, spectroscopic and mechanical properties, and nano- and mesoscale morphology – particularly in lower-dimensional materials and structures – and to enable burgeoning areas of user research. We define the cutting-edge of characterization not only by pushing spatiotemporal resolution and precision, but also by interrogating materials from complementary perspectives.



Mapping the 3-D location and identity of 23,000 atoms in an iron-platinum nanoparticle with atomic electron tomography [Nature 542, 7369 (2017)]

Unraveling the relationships between material composition, morphology, and function raises a number of fundamental scientific questions. For example, many of the synthesis efforts of Foundry users involve nonequilibrium systems that assemble dynamically and are responsive to changes in local environment. Experimental characterization, in tandem with theory and simulation, provides powerful insight, unraveling the nature of key properties at the nanoscale and drawing connections between these properties and materials composition and function. Importantly, these techniques are being developed with and made available to users worldwide to investigate the most important hard and soft materials, inorganic devices, biological systems, and complex hybrids with diverse functional interfaces: these include halide perovskites, 2D transition-metal dichalcoginide heterostructures, bio-inspired electrochemical membranes, functioning neurons, and more.

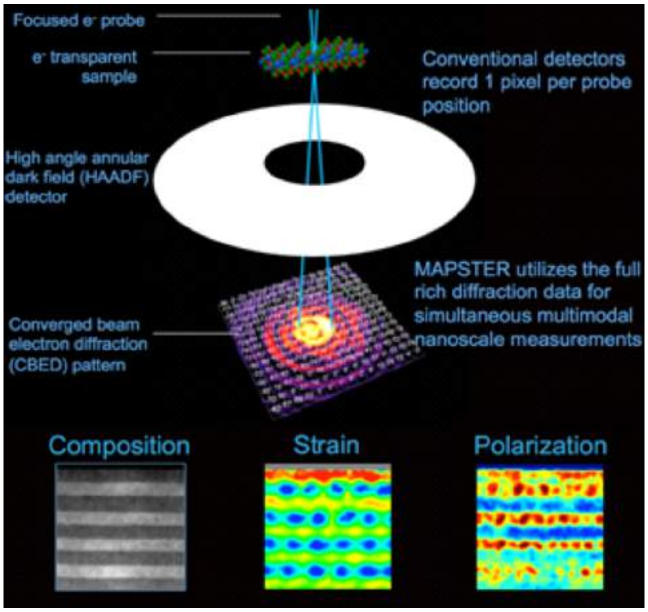
Future Directions

Imaging Function and Interactions in Buried Environments

In order to engineer revolutionary materials with new behaviors, we need first to understand the fundamental structure-property-function relationships in material and biological systems with abundant interfaces, and with interwoven heterogeneity and order on multiple length scales. For example, charge separation and migration in photovoltaic cells is dictated by the chemistry, structure, size and electrostatics of individual semiconductor grains, and the connectivity between them. Neurological function depends on real-time interactions of large sets of disparate cells in densely interconnected, widespread neural circuits. Systems engineered for catalysis, gas storage, and photoelectrochemistry also operate at complex heterogeneous interfaces between solids and gases or liquids. Currently there does not exist a complete set of imaging and localized spectroscopy techniques to enable probing of chemical reactivity at these interfaces. The goal of probing buried interfaces (e.g., well-beyond an extinction depth) also extends to the problem of nanoparticle nucleation or live cellular dynamics in liquid environments to enable imaging of individual components of nuclei or live cells with increasing speed and resolution.

Mapping of Fields in Space and Time

Multimodal Acquisition of Properties and Structure with Transmission Electron Reciprocal-space (MAPSTER) Microscopy takes advantage of advanced solid-state electron detectors to transform conventional TEM into multifunctional electron scattering beamlines, where multiple materials properties are mapped at the nanoscale from a single multidimensional dataset. MAPSTER acquires full 2D convergent beam electron diffraction (CBED) patterns at every beam position from a 2D atomic resolution raster scan (STEM) to produce massive 4-dimensional data sets (Figure 2). This full-field reciprocal space data contains localized information on sample structure, composition, phonon spectra, three-dimensional defect crystallography and hence, can generate simultaneously 2D maps of strain, polarization, local distortion and electric fields of materials at unit cell resolution (<1 nm). With MAPSTER Microscopy, the complexity and scale of TEM approaches the data richness of particle physics and astronomy, and we only begin to explore the manifold applications of mining such data.



We are developing the next generation of pixelated direct electron detectors in collaboration with Peter Denes (ALS) specifically designed for recording full electron diffraction patterns in scanning diffraction experiments. By optimizing pixel performance and incorporating on-detector processing electronics, we will record 100,000 diffraction frames per second, 100x faster than commercial devices. We are also working with both NERSC and ESnet in order to manage the extreme data rates up to 360 gigabits per second enabled by this technology. These detectors will directly benefit the full suite of scanning diffraction experiments described in this theme document including MAPSTER (at left), MIDI-STEM (see sidebar), and time-resolved strain mapping (above). This detector technology will also be applicable to HIRES ultrafast electron diffraction collaboration with Daniele Filippetto.

How materials interact with applied and internal fields is critical to the design and control of functionality. For example, detailed *in situ* analysis of the interactions of static and nanophotonic fields with materials and structures such as nanowires and core-shell nanoparticles could enable new technologies such as all-optical logic chips. Likewise, understanding the interaction of nanostructured defects in crystals or inhomogeneities in amorphous and heterogeneous materials relies critically on the ability to measure local strain *in situ* during deformation. Electron holography is also capable of mapping electric and magnetic fields at the nanoscale of both amorphous and crystalline materials. State-of-the-art energy resolved electron microscopy permits imaging of plasmon modes in nanomaterials, and integrated fiber-optics permits *in situ* pulsed-laser processing experiments as well as photoluminescence experiments. The development of new multimodal and multidimensional imaging techniques, such as MAPSTER, involve collecting radically new quantities of data—N-dimensional spectra—and we will address head-on the management, searching and indexing of this “big data.” Experimental development efforts involving spectroscopy in the time-domain will require significant developments in theory and simulation of excited states to model realistic pumped and/or probed excited states in nanoscale systems and at interfaces.

Planned Capabilities

Nanoscale Spectroscopic Imaging of Subsurface Interfaces and Defects

We will develop minimally invasive technologies able to probe the structure, electronics, and bonding of complex buried interfaces and deep-tissue biological structures, revealing previously unobserved and emergent functionality; additionally coupling with ALS-based efforts to study the entire span of mesoscopic time and energy scales.

We will couple recent breakthroughs in photoacoustic microscopy – which combines deeply-penetrating NIR excitation and acoustic response, even within dense, highly scattering media – with cutting-edge Foundry NIR nanocrystal probes, allowing us to understand the physical properties of matter at deeply buried structures and interfaces with nanoscale or subcellular resolution.

Energy conversion and transfer processes typically involve dynamics driven by nonequilibrium charge distributions created by photoexcitation. To explore and understand the bottlenecks in efficiency of such processes requires transient spectroscopies, ideally in combination with imaging techniques, to map and interpret dynamic process at relevant time scales. The techniques used and developed here will attract new communities of users and are synergistic with the research outlined in the Functional Nanointerfaces and Single-Digit Nanofabrication and Assembly theme documents, capturing the dynamics of charge separation, ion migration, gas flow, etc. these themes aim to control.

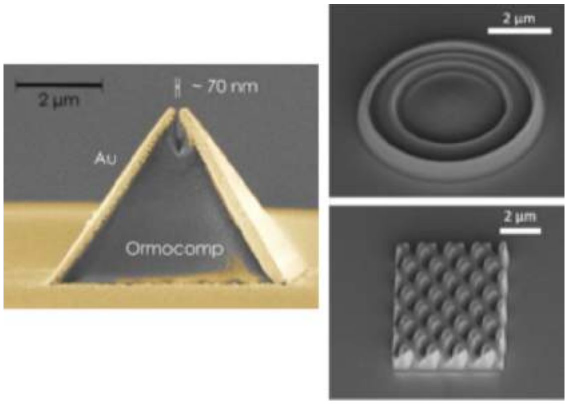
Multimodal High-Resolution In situ Transmission Electron Microscopy

Building off of the success of the TEAM project, and current efforts in atomic resolution tomography and *in situ* microscopy, the development of a multimodal *in situ* TEM will combine imaging with optical, X-ray, and electronic spectroscopies at atomic resolution under chemical, electrical, optical, thermal, magnetic and other stimuli. Multidimensional imaging of dynamic processes such as nucleation and transformation at the atomic scale will require dedicated electron microscopy instrumentation and technique development to increase image contrast, energy and time resolution, signal detection, sample environment, and probing capabilities. Development of advanced high speed electron detectors will push the limits of diffraction imaging techniques to allow for nanoscale mapping of structure and properties. Development of detector will enable ultrafast electron instrumentation for probing nanomaterial dynamics with dramatically decreased beam damage while source development will lead to probing of quantum phenomena and new techniques for spectroscopy. These developments will reinforce the strong position of our center at the forefront of electron microscopy, and strengthen our position for DOE goals outlined in its 2014 report on The Future of Electron Scattering.

Mapping Dynamics in Soft and Hybrid Materials

We plan to investigate exciton and photon transport using spatially independent excitation and probing with Localized Excitation Photo Current Microscopy (LEPCEM) and with combined cathodoluminesence excitation and near-field optical probing. Concomitantly, we will develop tools to watch biological, soft and hard material components as they dynamically combine and reorganize upon assembly with real-space *in situ* AFM/TEM and cryo-EM methods. Damage-free imaging is crucial here, so as not to affect assembly and dissolution pathways. We will build on our spin-polarized low-energy electron microscope (SPLEEM) expertise and instrumentation to image the distribution of charge and evolving transport pathways in soft and hybrid organic-inorganic semiconductor systems *in situ* and without damage. We will further develop near-real-time individual particle electron tomography with advanced electron detectors.

3.4 Single-Digit Nanofabrication and Assembly



Nano-optic devices creating using high-throughput nano-printing approach: Campanile probe (left), Fresnel lens (top), beam splitter (right). [Sci. Rep. 7, 1651 (2017), Nanotech. 27, 37, 375301 (2016), Opt. Lett. 41, 15 (2016)]

We use the term “single-digit nanofabrication (SDN) and assembly” to describe the structuring and characterization of materials whose key features are defined and resolved on a scale of 10 nm or less. Achieving this resolution in synthesis and fabrication is a central challenge of next-generation functional nanoscale and mesoscale materials. Addressing this challenge requires an understanding of the mesoscale coupling of atomic-scale interactions with assembly-scale manipulation and driving protocols. This knowledge is then used to create novel devices to promote breakthroughs in fundamental understanding and control in areas of technological interest such as quantum information systems, solar energy conversion, energy storage, light based communications, data storage, and catalysis. Building on the Foundry’s expertise in bottom-up (self-assembly) and top-down (lithography) nanofabrication – among the Foundry’s most heavily demanded capabilities – we will advance the forefront of fabrication. Major goals include addressing the grand challenges of 3D nanofabrication and understanding and controlling far-from-equilibrium guided assembly of multi-component systems composed of biological, organic, inorganic and hybrid materials.

Future Directions

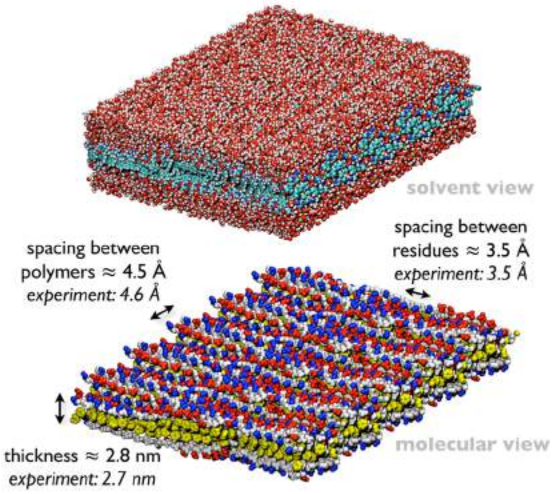
Precision Two-Dimensional Assembly

Foundry researchers continue to advance the science of ultrathin 2D assemblies of organic materials. These 2D polymers are assembled as discrete sheets, and are comprised of one or more monomer units. They exhibit both regular periodicity and long-range in-plane order. The connectivity between building blocks within each 2D organic layer can be either covalent or non-covalent. The layer thicknesses of these 2D structures are typically a few nanometers, corresponding to the size of a single molecule or a few well-packed molecules, and are generally several orders of magnitude smaller than the lateral dimension. The ability to synthesize precisely defined 2D organic layers is expected to extend the already rich functionality of conventional 1D linear polymers. Foundry scientists are making great progress in achieving better control of the design and synthesis of 2D structures, including control over the exact pore size, shape and functionality over a large area, and are engineering functionality in both homogenous and heterogeneous molecular nanosystems. Emerging applications of these materials include their use in membranes, storage materials, sensing, catalysis and optoelectronic devices.

Precision Three-Dimensional Nanofabrication

Combining traditional tools of top-down nanofabrication with directed self-assembly, we aim to create complex functional structures that are uniquely patterned in all three spatial dimensions with single-digit nanometer control enabled by bottom-up approaches. Such 3D structures and assemblies will open up new applications for guiding the flow of energy, light and chemical reactants and products. For instance, we will develop wafer scale processing of transition metal dichalcogenide heterostructures to build layered systems with engineered bandgaps that can direct electron flow. In addition, we will use sequential nanoimprint lithography with functionalized resist with precision alignment to create novel complex metamaterials and other light-guiding systems. We will create the highest quality scanning probes with new ion beam lithographies. Using novel scanning probes and two-photon lithography, we will explore new routes for writing 3D structures. The resultant fabricated 3D structures will, in some cases, act as both passive and active scaffolds to guide self-assembly in multiple dimensions, for instance to arrange di- and tri-block copolymers with other nano-objects.

Understanding and Controlling Heterogeneous Assembly far from Equilibrium

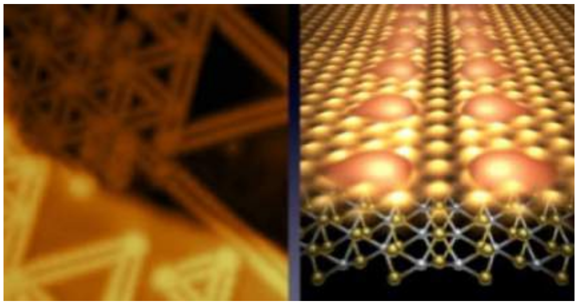


Atomistic simulations of peptoid nanosheets using the recently-developed MFToid forcefield [J. Comp. Chem., 35, 5, 360 (2014)] give nanosheet dimensions very close to those measured experimentally

While huge advances have been made in guided assembly of single component systems at or near equilibrium, forefront challenges are to understand and control the assembly of heterogeneous structures far from equilibrium. We will develop new theoretical approaches and fabrication strategies to understand how component shape, chemical functionality, chemical transformations and the flow of energy influence the organization of materials into structures far from equilibrium. In parallel, we will structure heterogeneous devices with controlled surface chemistry, topology and nm-scale feature sizes to replicate the virtual environments developed for simulation and theoretical modeling of assembly. Using multi-modal imaging techniques, we aim to observe assembly in real-time to validate and refine theoretical models. Fabricating assembly environments with more complexity, we can study how energy in the form of localized radiation, concentration and temperature gradients influence self-assembly. We already see potential applications of controlled far from equilibrium assembly. For instance, it is a route to overcoming roadblocks in areas such as semiconductor processing and data storage. We have an evolving relationship with industry to ensure adoption for rapid technological progress.

Planned Capabilities

Wafer scale processing of transition metal dichalcogenides (TMDs) by atomic layer deposition (ALD)



Linear defects in transition metal dichalcogenides create one-atom thick metallic wires that cross an otherwise intact semiconductor. [Nat. Phys. 12, 751 (2016)]

Two dimensional monolayer TMD films (e.g., MoS2, WS2, and MoSe2) have recently been shown to possess both high field effect mobilities and a direct band-gap in the visible, opening the possibility of exploring new classes of optoelectronic structures and basic physical phenomena. Currently, growth of these materials is limited to small crystals (100 µm) on flat substrates, greatly limiting both fundamental and application based experiments. We are currently investing in the development of a new type of TMD deposition process that uses ALD processes, maintaining the advantageous properties of ALD (scalability, conformality, and thickness and composition control). Transition metal oxide or nitride films are deposited by ALD, then converted through thermal or plasma annealing to their corresponding chalcogen (S, Se, Te). This opens the possibility of large area hetero-junctions (LED or photovoltaic applications) comprised of single or multi- TMD interfaces, TMD doping/alloying, and three-dimensional structuring of two-dimensional materials with growth over nano-fabricated surfaces, to name a few. These deposition and growth processes will open routes to new experimental interrogations ranging from fundamental physics to device applications at the wafer scale, and will draw a new user community to take advantage of this capability.

High-Resolution 3D Lithography and Precision-Aligned Nanoimprinting

Spatial resolution in multi-source ion beam lithography and deposition go far beyond that provided by electron beam and allow the direct patterning of materials in three dimensions. In addition, the system offers secondary electron imaging capabilities with improved resolution. A two-photon lithography system, modified to incorporate Foundry-developed sub diffraction limited nanooptics, would push the resolution of the 3D features into the single-digit nanometer range. Nanoimprint capabilities provide a means to replicate over-and-over single digit nano templates created using other lithographic techniques. With alignment, nanoimprinting will be expanded to fabricate integrated devices and complex 3-D structures and probes with high volume. In combination, this suite of technologies will be used to build probes for multimodal imaging and tip-based lithography, while its advanced imaging capabilities can be used to study and screen nanomaterials as part of the Foundry’s combinatorial efforts.

Simulation and Dynamic Imaging of Self-Assembly

Understanding the process of materials creation requires an ability to dynamically observe components as they combine and rearrange to produce a desired structure. To achieve these goals, real-space *in situ* AFM and TEM methods will be used, in tandem with far-from-equilibrium theories of self-assembly to guide the assembly of undriven systems that are prone to kinetic trapping (such as multicomponent mixtures), and of intrinsically nonequilibrium systems (such as those subjected to spinning and drying). Visualization tools include our multimodal imaging methods, particularly the 3D tomographic methods that build on the extraordinary performance of existing aberration-corrected electron microscopes and the gentle cantilevers for *in situ* high resolution imaging. We will further develop multiscale simulation tools to model and thereby infer structure across multiple length scales from time-dependent scattering measurements at the ALS. Such interpretation will allow new understanding of the dynamic “pathways” by which materials assemble.

4. Strengthening Scientific and User Resources

Above, several strategic scientific priorities were identified that will expand the productivity, efficiency and utilization of the Molecular Foundry. In order to pursue these promising opportunities in nanoscience over the next five years, the center will seek to retain and recruit outstanding scientific, technical and administrative staff, and continue to develop its suite of state- of-the-art instrumentation.

The Foundry’s four scientific themes are designed to connect current expertise and instrumentation with the needs of users. Each theme contains two distinct future directions that serve to guide the Foundry over the next five years and the capabilities required to achieve them. In the section that follows, two tables list resources – expertise and equipment – that will allow these capabilities to grow and enhance the effectiveness of Foundry research. Personnel and instrument capabilities that are of high demand by Foundry users, and are essential to existing and new research efforts, were identified for reinvestment. The tables map each resource to the four themes, indicate if they are a new need or reinvestment, and assign a rough timeline for investment (short term=1-3 years; long term=3-5 years). Finally, organizational enhancements designed to maximize the User Program’s exposure and operational efficiencies are described.

Given limited resources, these lists are meant to guide our priorities, initiatives and investments in the future, but since they do not attempt to include every future capability, the lists maintain the flexibility required to evolve and react to changing needs of the larger scientific community.

4.1 Enhancement of Foundry Expertise

A major part of the Foundry’s success has been the emergence of outstanding scientific staff that are seen by many in the general scientific community as the main draw to the Foundry. The maintenance of diverse, high-quality expertise among Foundry staff enables world-leading research and attracts top scientific talent as users.

In FY 2016, the Molecular became an independent division at Berkeley Lab that led to the creation of the current operational structure. In addition, the Molecular Foundry has launched several new recruitments in the last year for scientific and technical staff. Most notably, a search is underway for the next director following the promotion of Jeff Neaton to Associate Laboratory Director of the Energy Sciences Area, which oversees the Foundry, as well as the ALS, Materials Sciences and Chemical Sciences division. Current recruitments are included in the table below.

In 2015, the Foundry launched its Theme Postdoc Program that supports theme-based teams of three multidisciplinary postdocs for two years. This program is designed to further enable and encourage the multidisciplinary research described in this Strategic Plan through investments into the Foundry’s collaborative themes rather than its technical facilities. Now in its third year, the program consists of three cohorts:

- Cohort 1 (Interfaces): Design & Growth of Wide-Area and Conformal Transition Metal Dichalcogenide Heterojunctions
- Cohort 1 (Multimodal): Direct Structural Determination of Soft & Hybrid Nanostructures with a Structured Phase Electron Beam (MIDI-STEM)
- Cohort 2 (Combi) A Combinatorial Approach to Multifunctional Porous Graphitic Materials (PGMs)
- Cohort 2 (Single-Digit Nano): Quantum-Confining Metal-Organic Chalcogenide Assemblies (MOCHAs) for Energy Transport and Photonics
- Cohort 3 (Interfaces): Harnessing Responsive and Reconfigurable Organic-Inorganic Nanointerfaces for the Synthesis of Metastable Quantum Materials and Systems

Cohort 3 (Multimodal): Coherent Single-Electron Source for Quantum Microscopy and SpectroscopyAlso in 2015, the Molecular Foundry began a partnership with the ALS to enhance scientific collaboration and provide a more integrated experience for users who were seeking resources from both user facilities. This investment included support to develop greater automation and throughput for the SAXS/WAXS beamline along with a jointly funded project scientist. Following the conclusion of this successful experiment, both organizations are looking for new ways to continue this collaboration. While proposals are still being considered, it is likely that some shared personnel will be involved.

Despite these recent investments, new vacancies have emerged with the departure of several staff and project scientists, as well as the identification of new areas of need. The list below represents a combination of existing vacancies and anticipated priorities.

Expertise	Combinatorial	Interfaces	Multimodal	Single-Digit Nano	Short Term	Long Term
Director	x	x	x	x	x	
Staff scientist, Organic	x	x		x	x	
Staff scientist, Theory	x	x	x	x	x	
Staff scientist, Nanofabrication		x	x	x	x	
Technical staff, Nanofabrication		x	x	x	x	
Technical Staff, NCEM		x	x		x	
Technical staff, Imaging	x	x	x	x		x
Joint Foundry/ALS project scientist	x	x		x		x

4.2 Enhancement of Equipment Resources

In addition to the expertise of Foundry staff and multidisciplinary training and collaboration opportunities, the Foundry offers users access to state-of-the-art instrumentation that leads to groundbreaking research. Keeping equipment current and anticipating trends in user demand is essential for the Foundry to maintain its position as a leading nanoscience center and to take advantage of the scientific opportunities within reach of Foundry scientists and users.

In the last year, several major investments were made to renew and expand our physical resources. Highlights include: tabletop SEM, XPS, TGA, EM tensile holder, continued development of the HERMAN reactor, in situ TEM, sample prep FIB, additional compute nodes, next generation DED wiring, microfluidics work area, photocurrent AFM upgrade, quantum efficiency station, table top powder XRD, and a spectrometer upgrade.

This table identifies high-priority areas of need based on current user demand and the instruments required to achieve the goals outlined in this document.

Equipment	Combinatorial	Interfaces	Multimodal	Single-Digit Nano	Reinvestment	New, Short Term	New, Long Term
ALD station for novel metal chemistries	x	x		x		x	
e-Beam Writer		x	x	x	x	x	
EELS Spectrometer	x	x	x	x		x	
Gel permeation chromatography (GPC)	x	x		x	x	x	
MALDI	x	x			x	x	
Microfluidic synthesis and characterization suite	x		x	x		X	
Microspotting Robot	x	x				x	
Single-crystal XRD	x	x				x	
Super-resolution Microscope	x		x	x		x	
Solid-state NMR	x	x	x			x	
Multi-source ion beam lithography system			x	x	x		x
e-Beam Evaporator		x	x	x	x		x
In situ liquid/gas cell TEM sample holder	x	x	x				x
Fast piezo AFM stage	x	x	x	x			x
Nanoimprinting with high-precision realignment		x	x	x	x		x
High-performance compute cluster	x	x	x	x	x		x
Two-photon lithography		x	x	x			x
MAD-LEEM: Dynamics of surface magnetism, damage-free imaging of soft matter, phonon-resolution spectroscopy		x	x				x
Quantum Multi Pass Electron Microscope	x	x	x	x			x
1K TEM	x	x	x	x			x

4.3 Enhancement of User Outreach, Engagement, and Services

In concert with enhancements to the expertise and equipment offered at the Foundry, efforts are made to continually seek to actively grow and strengthen the user community, while improving services to current and prospective users. Looking forward, the organization will focus on four priority areas, detailed below.

Minimize Bias in the User Program and Foundry Research Environment

In collaboration with the company AcuityWorks, the Foundry has worked to identify aspects of the User Program that could be more vulnerable to bias, and thereby negatively impact user access to the facility, limit our ability to identify the strongest user research proposals, prevent us from building a geographically diverse user base, and limit the productivity of collaborative research. Areas where we intend to focus efforts are: more broadly advertising the User

Program opportunity; ensuring that first-time users are able to write a strong proposal without the help of a Foundry PI; ensuring Foundry User Program goals are reflected in the proposal review criteria; helping new users learn the ropes; and creating well-distributed policies that describe and reward collaborative practices.

Build and Promote a Culture of Safe and Collaborative Science

The Foundry's culture of safe and collaborative science is one of our most valuable assets, underpinning all of our scientific and programmatic successes. We will continue to build and promote that culture in the coming years through a number of activities, and aim to be the gold standard that users look towards when they return to their home institutions. The Foundry's Safety Committee continues a tradition of engagement across all facilities through its prioritization of integrated safety management. Safety is included in everything that is done at the Foundry, and the daily attention to best practices culminates in the annual Safety Retreat where users and staff come together to reaffirm the commitment to a safe work environment, while also innovating the way that safety can enhance – rather than get in the way of – research.

The Foundry's Diversity and Inclusion Committee focuses on nurturing and expanding the open culture at the Foundry, and hosts a number of workshops each year on topics like micro-aggressions in the workplace and intercultural communication. Similarly, the efforts of the Foundry's Career Development Committee will help promote collaborative science through planned activities like a panel discussion on building user collaborations. Both committees were formed in 2016 following the establishment of the Molecular Foundry as an independent division at Berkeley Lab and members regularly assist in the development of new operational policies and resources for staff and users that bring these core values to the fore in everything that we do.

A recent survey of users found that they were very satisfied with the Foundry's culture but there are gaps in communication of activities and resources. In response, we will prioritize efforts to provide greater guidance and information dissemination both in person and electronically via the website and the newly launched newsletter. We will also continue our close collaboration with the UEC and integrate users into various committees including staff search committees and those listed above.

Improve Performance Metrics for Industry Users

The Molecular Foundry has a strong and growing engagement with industry (~13% of user projects in FY 2017), and it remains a priority to address the challenge of assessing the impact of industry user projects. Efforts are underway to implement a broader set of metrics for evaluating industry user proposals, including IP development and fund raising. Users on industry proposals will be asked to report these outcomes in addition to the general reporting requirements at project completion. The outcomes will be provided to the proposal review board (which is generally 15-20% from industry) as part of any future proposal submissions from a given industry user to help provide greater context when evaluating the impact of proposed work. These metrics will also be shared with DOE during program evaluation. Internally, these performance metrics will help guide policy development and resource allocation.

Expand Partnerships and Leverage with Local Environment

The Molecular Foundry will continue to explore new ways to ensure that it capitalizes on its local scientific environment within LBNL and the Bay Area. We are engaged in discussions with the ALS about ways to improve coordination of our joint access arrangement, which provides

Foundry users with access to ALS beamtime through their Foundry proposal and provides Foundry access for ALS users in support of their ALS work. Efforts are underway to increase the visibility of Foundry capabilities available to ALS users and to cultivate cross-pollination of various local research communities through joint seminar series, invited talks, and workshops. We are also revamping the Foundry’s Affiliate Labs program. New partnerships are being built through this program with groups such as the Advanced Biofuels Process Demonstration Unit and the Center for X-Ray Optics.