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Nanotechnology institutions

Research opportunities at the Molecular Foundry

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Abstract

The Molecular Foundry is a Department of Energy-funded Nanoscale Science Research Center (NSRC) providing support to researchers from around the world. Nanoscience has the potential to open new frontiers in energy, electronics, materials science and healthcare. Research conducted at the Molecular Foundry identifies these new frontiers and develops science and technology strategies to enable them. Organized into six interdependent research facilities, the Foundry and its affiliated research laboratories provide access to state-of-the-art instrumentation, scientific expertise and specialized techniques to help users address myriad challenges in nanoscience and nanotechnology.

Keywords: energy; nanostructures; user facility.

1. Overview

Capitalizing on the fundamental differences in physical, chemical and biological behavior of materials at dimensions between molecular and bulk systems, nanoscience examines the compelling and singular properties found neither in atoms and molecules, nor at macroscopic dimensions. Such unique properties have already improved routine commercial products such as sunscreen and stain-resistant clothing, and hold promise for uncovering new materials with applications in energy, security, agriculture and healthcare.

Ideally, nanoscale materials combine advantageous features of bulk and molecular systems into materials that can be readily designed, manufactured and integrated into functional devices. Therefore, the design and manufacture of structures at nanometer dimensions requires innovations in materials synthesis, physical patterning, structural characterization and theory, encompassing disciplines such as biology, chemistry, physics and engineering. As such, scientists around the world are actively seeking and testing "top-down" and "bottom-up" strategies to engineer nanostructures [1] that can interface with macroscopic materials and can be scaled up to manufacture devices for real-world applications.

"Top-down" strategies make use of advanced lithography, electron-beam writing and nanoimprinting techniques to directly generate a pattern into a substrate. These techniques, owing to their historical origin, are particularly fruitful in developing metal- and semiconductor-based nanostructures. "Bottom-up" methods exploit atoms and molecules that spontaneously assemble into organized structures, without human intervention [2]. Commonly employed by nature, self-assembly of materials occurs at length scales ranging from cellular components to star-studded galaxies. This tactic is particularly useful for constructing systems, particularly biological, organic and other soft materials, with nanoscale precision, particularly for structures below the optical diffraction limit [3].

By combining "bottom-up" and "top-down" strategies, scientists can integrate nanosystems and tailor materials to achieve a specific application. However, as the dimensions of a material decrease, special consideration must be taken to understand the size-dependent properties of a material within the context of a given application, while optimizing molecular and materials design [4]. For example, optical properties originate from the band structure of a nanoscale material, whereas magnetic properties are dominated by the exchange interactions between spin states [5].

It is probable that both "top-down" and "bottom-up" methods will need to work in concert with larger-scale components in functional devices [1]. This also requires examining nanomaterials with high precision to tease out structure-property relationships. In addition, the advent of techniques for atomic scale imaging, such as scanning tunneling microscopy and atomic force microscopy, along with advances in traditional electron microscopy, have greatly aided efforts to view nanoscale structures and their modification under external perturbation [6].

2. Nanoscale Science Research Centers

The United States has invested significant resources into nanoscience and technology research and development. This can be evidenced by the 2001 National Nanotechnology Initiative, which pools the collective efforts of 15 United States federal agencies broadly involved in nanoscience and nanotechnology, from fundamental research to regulation and commercialization (FY 2011 budget: $1.8 billion) [7]. In support of the National Nanotechnology Initiative, the US Department of Energy's Scientific User Facilities Division, for example, has developed and launched five new Nanoscale Science Research Centers (NSRCs) to support the synthesis, processing, fabrication and analysis of materials at the nanoscale.

Figure 1 The Molecular Foundry at Lawrence Berkeley National Laboratory is a Department of Energy-funded program providing support to researchers from around the world whose work can benefit from or contribute to nanoscience (image courtesy of Roy Kaltschmidt).

These centers are designed to be premier user centers for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools and new computing capabilities. Together, the NSRCs provide a gateway to other major user facilities for X-ray, neutron and electron scattering. Each nanoscience user facility contains clean rooms, laboratories for nanofabrication, one-of-a-kind signature instruments and other tools (e.g., nanopatterning instruments and research-grade probe microscopes).

These facilities provide researchers from around the world free access to state-of-the-art instrumentation, computational methods and expert scientific staff – a novel and standalone setting designed to promote collaborative work among scientists from varied disciplines including chemistry, biology, physics, materials science, engineering and computer science.

In particular, the Molecular Foundry at Lawrence Berkeley National Laboratory (Figure 1) is a Department of Energy-supported NSRC dedicated to fostering discovery and technology development in nanoscience in a safe working environment. The mission of the Foundry is to provide its community of users with access to state-of-the-art instrumentation and expert staff to advance their research interests in the synthesis, characterization and theoretical analysis of nanostructures. Users come from academic, industrial or 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 proposal review process.

Scientists sharing common technical interests are in the six technical facilities of the Foundry:

- Imaging and manipulation of nanostructures
- Nanofabrication
- Theory of nanostructured materials

Box 1 Nanocomposite for high-capacity hydrogen storage (Figure 2).

A new composite material for hydrogen storage consisting of magnesium nanoparticles sprinkled through a polymer matrix was recently designed at the Molecular Foundry [8]. This pliable nanocomposite rapidly absorbs and releases hydrogen at modest temperatures without oxidizing the metal after cycling – a major breakthrough in materials design for hydrogen storage, batteries and fuel cells.

For hydrogen to be a viable fuel source, it must be safely stored, yet readily released upon heating. Limited by materials unable to leap these conflicting hurdles, hydrogen storage technology has lagged behind other clean energy candidates. Previous studies attempted to address both issues by locking hydrogen into solids through strong chemical bonds, packing larger quantities into smaller volumes with low reactivity. However, current materials can only absorb a small amount of hydrogen and require extreme heating or cooling to boost overall energy efficiency.

In this new nanocomposite, 4 wt.% hydrogen is rapidly absorbed and maintained at 200°C. The team also tracked defects within individual magnesium nanocrystals, providing unprecedented views into the atomic and nanoscale structure of this new class of hydrogen storage materials.

Box 2 Self-assembly of “molecular paper” (Figure 3).

Researchers at the Molecular Foundry have developed a “molecular paper” material [9] whose properties can be precisely tailored to control the flow of molecules, or serve as a platform for chemical and biological detection. Two-dimensional nanosheets are commonly employed in biological systems such as cell membranes, and their unique properties have inspired interest in materials such as graphene. This entirely new material mirrors the structural complexity of biological systems with the durable architecture needed for membranes or integration into functional devices.

These self-assembling sheets are made of peptoids, engineered polymers that can flex and fold like proteins while maintaining the robustness of manmade materials. Each sheet is just two molecules thick yet hundreds of square micrometers in area – akin to “molecular paper” large enough to be visible to the naked eye. What’s more, unlike a typical polymer, each building block in a peptoid nanosheet is encoded with structural “marching orders” – suggesting its properties can be precisely tailored to a variety of applications in device fabrication, nanoscale synthesis and imaging.

Box 3 Nanocrystal coatings for smart windows (Figure 4).

Molecular Foundry scientists have unveiled a semiconductor nanocrystal coating material capable of controlling heat from the sun while remaining transparent [10]. Based on electrochromic materials, which use a jolt of electric charge to tint a clear window, this breakthrough technology is the first to selectively control the amount of near infrared radiation without affecting its visible transmittance. Such a dynamic system could add a critical energy-saving dimension to “smart window” coatings.

The team developed a nanocrystal film of electrically doped indium tin oxide, a transparent semiconductor typically used as a conductive coating for flat screen TVs. By manipulating the electrons within this semiconducting film, they could tune the collective oscillations of these electrons – a phenomenon called plasmonics – across the near infrared frequency range.

Dynamic window coatings could translate into significant energy savings in buildings: computer simulations of building performance suggest smart window coatings could offset the use of climate control and illumination systems by up to 50% [11]. These findings represent a step towards an ideal smart window, which would be able to selectively choose which region of sunlight is needed to optimize the temperature inside a building.

Box 4 Bringing plasmonic nanofields into focus (Figure 5).

A research team at the Molecular Foundry demonstrated an innovative imaging concept to visualize plasmonic fields from devices with nanoscale resolution [12]. In plasmonic devices, electromagnetic waves crowd into tiny metal structures, concentrating energy into nanoscale dimensions. This savvy coupling of electronics and photonics could be harnessed for high-speed data transmission or ultrafast detector arrays.

However, studying plasmonic fields in nanoscale devices presents a real roadblock for scientists, as examining these structures inherently alters their behavior. Previously, the team engineered bowtie-shaped plasmonic devices to steer light at the nanoscale. These nanocolor sorter devices focus and sort light in tiny spaces to a desired set of colors or energies – crucial for detectors.

Currently, by imaging fluorescence from gold within a bowtie and maximizing the number of photons collected, the team gleaned the position of plasmonic modes – oscillations of charge that result in optical resonance – just a few nanometers apart.

In parallel, the team developed a web-based toolkit designed to calculate images of plasmonic devices to simulate how changing the size and symmetry of a plasmonic antenna affects its optical properties. This toolkit is freely available for other researchers to download on nanoHUB.org, a computational resource for nanoscience and technology.

- Inorganic nanostructures
- Biological nanostructures
- Organic and macromolecular synthesis

These facilities are outfitted with state-of-the-art, often one-of-a-kind instrumentation and staffed with world-class scientists with expertise in the specific technical areas. Users’ projects generally involve multiple facilities, further enhancing interactions across the six facilities of the Foundry.

3. Research themes

Foundry scientists’ internal research converges around four research themes to reflect the expertise of the Foundry staff:

Combinatorial nanoscience – using robotic synthesizers to generate and test large libraries of biological and inorganic nanostructures using highly automated, parallel processes. This allows researchers to rapidly test thousands of compounds for sought-after optical, electronic and thermal properties.

- Nanointerfaces – engineering the mechanical and transport properties of hybrid nanomaterials (materials with differing properties, e.g., inorganic nanomaterials and complex living organisms). This is accomplished through synthesis of heterostructures and interfaces, first-principles simulations and characterization of function.
- Multimodal *in situ* nanoimaging and spectroscopy – applying multiple imaging techniques, including scanned probe

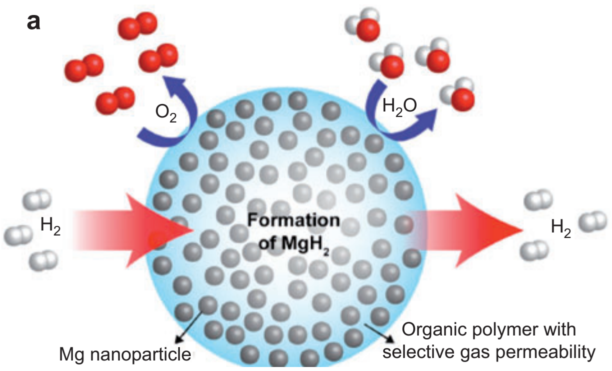

Figure 2 (Box 1) Schematic illustration of high-capacity magnesium nanocrystals encapsulated by a selectively gas-permeable polymer matrix to create a new and revolutionary hydrogen storage composite material (image courtesy of Jeff Urban).

microscopy, nanophotonics and electron microscopy, to investigate dynamic nanoscale phenomena in liquid and vapor environments. There is a strong emphasis on soft materials.
- Single-digit nanofabrication – using biological and organic templates, advanced lithographic techniques and probe-based surface modification to fabricate nanoscale structures, features and spaces that measure >10 nm.
- Since its inception in 2006, many exciting discoveries have emerged from user and internal research at the Molecular Foundry (Boxes 1–4, Figures 2–5).

These four themes by no means encompass the breadth of research conducted at the Foundry; indeed, many Foundry scientists are actively involved in a number of larger efforts at Lawrence Berkeley National Laboratory and the University of California, Berkeley. These efforts include the Department of Energy's Joint Center for Artificial Photosynthesis, Center for Nanoscale Control of Geologic CO_2 and Center for Gas Separations Relevant to Energy Technologies. These efforts are part of a broader initiative at Lawrence Berkeley National Laboratory for global low-carbon energy system and an initiative to accelerate discovery and innovation, called Carbon Cycle 2.0.

4. Conclusion

The Molecular Foundry and other NSRCs exemplify the type and scale of interdisciplinary settings needed to tackle large-scale scientific challenges, such as our current and future

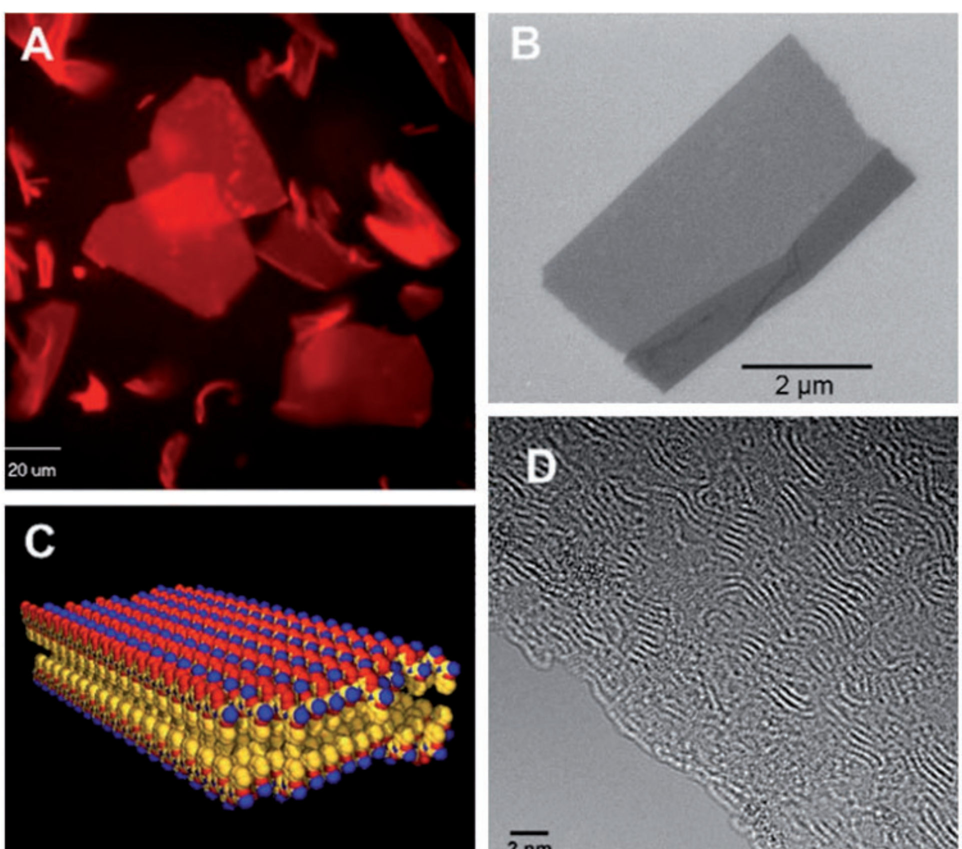

Figure 3 (Box 2) Imaging (A, B, D) and schematic (C) of two-dimensional crystalline sheets assembled from peptoid polymers into a "molecular paper" material (image courtesy of Ron Zuckermann).

Figure 4 (Box 3) Molecular Foundry researchers have unveiled a semiconductor nanocrystal coating material capable of controlling heat from the sun while remaining transparent. This heat passes through the film without affecting its visible transmittance, which could add a critical energy-saving dimension to "smart window" coatings (image courtesy of Delia Milliron).

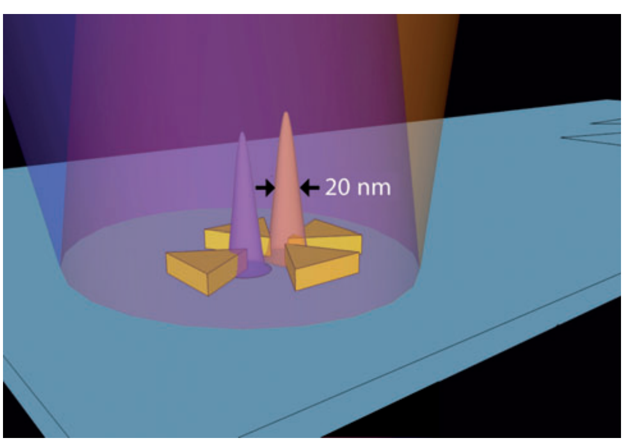

Figure 5 (Box 4) Schematic of fluorescence from gold within a bowtie-shaped plasmonic device to glean the position of plasmonic modes just a few nanometers apart. This open source, web-based imaging toolkit developed at the Molecular Foundry is designed for researchers studying plasmonic and photonic structures (image courtesy of Alexander Weber-Bargioni).

needs for carbon-neutral and renewable energy sources. Indeed, these centers have accelerated efforts in developing nanotechnology for renewable energy collection and conversion, biomimicry and imaging.

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