

# UNLOCKING NEW SCIENTIFIC AND TECHNOLOGICAL FRONTIERS

The Center for Nanoscale Materials at Argonne National Laboratory **The Center for Nanoscale Materials** (CNM) a U.S. Department of Energy (DOE) Office of Science user facility — is located at Argonne National Laboratory, just 30 minutes from Chicago. Academic, industrial and international researchers can access the center through our user program for both proprietary and non-proprietary research. There is no cost to use the CNM if the research is intended for the public domain.



NANOPHOTONICS AND BIOFUNCTIONAL STRUCTURES



QUANTUM AND ENERGY MATERIALS



NANOFABRICATION AND DEVICES



ELECTRON AND X-RAY MICROSCOPY



THEORY AND MODELING

We offer more than 100 tools and capabilities. From X-ray microscopy to cleanroom-based nanofabrication techniques, the CNM provides researchers with a powerful combination of scientific resources found nowhere else. The CNM is one of the DOE Office of Science Nanoscale Science Research Centers, constructed under a joint partnership between DOE and the State of Illinois.

# USER COMMUNITY

#### **CALLS FOR PROPOSALS**

We issue three calls for user proposals each year. These brief, two- to three-page proposals are due in March, July and October.

An external **Proposal Evaluation Board** reviews user proposals. Approved projects are granted access to CNM facilities for a maximum of one year.

#### SAFETY

Safety is an essential part of all work done at CNM. Users are properly trained before working in our facilities.

We provide a variety of resources and networking opportunities designed to make users' time with us productive and memorable.

#### **USER RESOURCES**

Bi-weekly colloquium series
 CNM hosts guest speakers
 from around the world to talk
 about cutting-edge research.
 The colloquium series provides
 a forum for multidisciplinary talks
 and fosters interactions with
 facility users and CNM staff.

Seminars

We host regular seminars to enhance multidisciplinary collaboration.

User Executive Committee (UEC)
 The UEC serves as an advocacy
 group for the CNM user community
 and advises the CNM Director on
 user priorities. The UEC is also
 responsible for organizing the
 scientific content of the annual joint
 Advanced Photon Source (APS) and
 CNM Users Meeting.

APS/CNM Users Meeting
 This event attracts 400+ researchers
 and 50+ vendors each year. It
 includes technical workshops,
 plenary and poster sessions, social
 events and short courses. A Best
 Student Poster Award competition
 is held for students at CNM.

 Women in Science and Technology (WIST)

This Argonne program aims to promote the success of women in scientific and technical positions. All individuals are welcome to participate.







### Global Demographics



#### U.S. Demographics



CNM By the Numbers



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# LOOKING AT CLOSE PACKING OF QUANTUM DOTS



A typical transmission electron microscopy (TEM) image of truncated-tetrahedral quantum dots.



On the left, a computer model depicts a selfassembled tetrahelix made up of tetrahedral quantum dots, made of cadmium and sulfur (or elements related to sulfur), and on the right, a skeleton view of the tetrahelix demonstrates the chiral structure of the assembly.

**THE IMPETUS** Mathematicians have long been interested in the ways in which shapes pack against one another to fill a three-dimensional volume. In a new experiment, scientists observed the packing behavior of truncated tetrahedral quantum dots.

The assembly of uniform nanocrystal building blocks into well-ordered superstructures is a fundamental strategy for the generation of meso- and macroscale metamaterials with emergent nanoscopic functionalities. Using self-assembly methods, scientists at the CNM, with collaborators from Brown University, Cornell University and Germany (the Max Planck Institute and Heinrich Pette Institute in Leibniz, and Institute for Experimental Virology in Hamburg), produced and observed single-component tetrahedral building blocks in three distinct complex superstructures, including a one-dimensional chiral tetrahelix.

**THE WORK** Using techniques in real and reciprocal spaces, scientists successfully characterized the superstructures from their nanocrystal translational orderings down to the atomic-orientation alignments of individual quantum dots.

The superstructures were created by drop-casting a solution of truncated tetrahedral quantum dots in hexane onto a transmission electron microscopy grid placed on a silicon wafer. The truncated tetrahedral quantum dots in solution self-assembled into one, two and three dimensions with one common structural feature: preferred facet-to-facet alignment.

Scanning transmission electron microscopy (STEM) and STEM-energy dispersive X-ray spectroscopy (EDS) mapping were performed at CNM.

**THE IMPACT** The observations expand the collection of superstructures that can use tetrahedral building blocks. The findings also bring the spontaneous formation of nanocrystal assemblies to a higher level of complexity, including chirality in some cases.

Y. Nagaoka, R. Tan, R. Li, H. Zhu, D. Eggert, Y. A. Wu, Y. Liu, Z. Wang and O. Chen, "Superstructures Generated from Truncated Tetrahedral Quantum Dots," *Nature* 561, 378 (2018).



#### REVEALING THE INTRINSIC NATURE OF **QUANTUM TRANSITIONS IN NON-CLASSICAL PHOTON SOURCES**



Simulated excitation pattern of an emitter dipole shows uniform absorption.



Electric field distributions show the likelihood of optical transitions for light polarized along the short axis (left) is lower than along the long axis (right).

**THE IMPETUS** Scientists at the CNM with collaborators from the University of Chicago and Northwestern University have shown how polarized single photon emission from semiconductor nanoparticles can be achieved despite their two-dimensional isotropic emission dipoles.

Quasi-two-dimensional nanoplatelets (NPLs) possess extremely narrow spectral features due to their near-perfect monodispersity in the quantum-confined thickness dimension. NPL-based optoelectronic devices are promising for highly efficient dipole coupling and energy transfer processes. NPLs are also potentially interesting candidates for single photon sources in quantum information processing.

To leverage these exceptional properties of NPLs for high-performance optoelectronic and quantum photonic applications, knowledge of their transition dipole moment is essential for efficient dipole-dipole and dipole-cavity mode coupling.

**THE WORK** The research team investigated individual quasi-two-dimensional NPLs using higher-order laser scanning microscopy and found that absorption dipoles in NPLs are isotropic in three dimensions at the excitation wavelength. Correlated polarization studies of the NPLs reveal that their emission polarization is strongly dependent on the aspect ratio of the lateral dimensions.

The research team concluded that emission dipoles in NPLs are isotropic in the plane of the NPLs. The study presents an approach for disentangling the effects of dipole degeneracy and electric field renormalization on emission anisotropy and can be adapted for studying the intrinsic optical transition dipoles of various nanostructures.

**THE IMPACT** The study will further enable quantum optics and quantum network opportunities utilizing nanoscale single photon emitters by manipulating their emission polarization and directionality.

X. Ma, B. T. Diroll, W. Cho, I. Fedin, R. D. Schaller, D. V. Talapin and G. P. Wiederrecht, "Anisotropic Photoluminescence from Isotropic Optical Transition Dipoles in Semiconductor Nanoplatelets," *Nano Letters* 18, 4647 (2018).



#### THROUGH MACHINE LEARNING, **NEW MODEL HOLDS WATER**



Nucleation simulations of ice using a machinelearned-BOP model. MD simulation snapshot at 230 ns shows various stages of grain growth and grain boundary during post-nucleation. Blue, brown and green spheres = cubic, hexagonal and amorphous ice (liquid water omitted for clarity).



Molecular dynamics simulations based on machine-learning show how grains of ice form and coalesce in supercooled water, which results in ice with imperfections. These simulations help scientists learn about the movement of the boundary between ice grains (yellow/green/ cyan) and the stacking disorder that occurs when hexagonal (orange) and cubic (blue) pieces of ice freeze together. This information is important in applications such as climate modeling and cryogenics. These simulations were performed on two supercomputers: Mira at the Argonne Leadership Computing Facility, and Carbon at the Center for Nanoscale Materials. **THE IMPETUS** While water is perceived to be one of the simplest substances in the world, modeling its behavior on the atomic or molecular level has frustrated scientists for decades. To date, no single model has been able to accurately represent the plethora of water's singular characteristics, including the fact that it is densest at a temperature slightly higher than its melting point.

Researchers at CNM, together with CNM users from Argonne, the University of Louisville and the University of Chicago, achieved a breakthrough in the effort to mathematically represent how water behaves. To do so, the team used machine learning to develop a new, computationally inexpensive water model that more accurately represents the thermodynamic properties of water, including how water changes to ice at the molecular scale.

**THE WORK** Trying to create quantum mechanical or atomistic models to capture water's behavior had flummoxed researchers because they are so computationally intensive and still fail to reproduce many temperature-dependent properties of water.

The team used the high-performance computing resources of the Carbon cluster at CNM, the Mira supercomputer at the Argonne Leadership Computing Facility, a DOE Office of Science user facility, Fusion at Argonne's Laboratory Computing Resource Center, and the National Energy Research Scientific Computing Center, to perform simulations of up to 8 million water molecules to study the growth and formation of interfaces in polycrystalline ice.

To achieve the high accuracy of the coarse-grained model, the researchers trained the model using information drawn from nearly a billion atomic-scale configurations involving temperature-dependent properties that are well known.

**THE IMPACT** This new model, termed "coarse-grained," achieves a fidelity on par with models that incorporate an atomic-level description. For the researchers, the choice to use entire water molecules as the fundamental unit in the model allowed them to perform the simulation at low computational cost. The researchers also showed that their approach could be used to improve the performance of other existing atomistic and molecular models.

H. Chan, M. J. Cherukara, B. Narayanan, T. D. Loeffler, C. Benmore, S. K. Gray and S. K. R. S. Sankaranarayanan, "Machine Learning Coarse Grained Models for Water," *Nature Communications* 10, 379 (2019).



#### INVESTIGATING DYNAMICS BEHIND **SHEAR THICKENING** IN FLUID FLOW



Small angle X-ray scattering patterns measured for a monodisperse colloidal fluid at different oscillatory shear stresses at 1 Hertz. **THE IMPETUS** What do paint, dishwasher detergent and blood have in common? All are composed of particles suspended in a carrier liquid, flow when stirred or forced, but remain thick at rest. This behavior in complex fluids is called shear thinning: their viscosity decreases during mixing and increases at rest. But certain fluids, when the mixing speed increases, can pass through the region of shear thinning and move into a region where viscosity increases dramatically. This effect, known as shear thickening, has been under investigation for several decades as engineers sought to solve complex production problems caused by the phenomenon.

**THE WORK** When fluids are mixed at low speeds, the suspended particles form ordered layers that can slide easily across each other, facilitating flow—but when exposed to high speeds, the layers become disordered and stumble over one another, hindering flow. This change in the type of flow is called "order-to-disorder transition."

An Argonne team of nanoscientists and physicists has unraveled this mystery by studying a shear-thickening fluid with in situ X-ray characterization.

Using the rheometry small-angle X-ray scattering technique at Argonne's Advanced Photon Source, a DOE Office of Science user facility, and co-managed with the CNM, Argonne researchers measured how the nanoparticles flowed in response to an applied force in real time.

**THE IMPACT** The highly uniform suspensions created by the team allowed separation of the two phenomena: order-to-disorder transition and normal shear thickening. Until now, they had been indistinguishable in other experiments. These behaviors are driven by two separate, independent mechanisms.

Researchers are now seeking to understand the mechanism that really contributes to shear thickening. These studies could lead to applications in three-dimensional printing, the chemical industry and the biomedical field.

J. Lee, Z. Jiang, J. Wang, A. R. Sandy, S. Narayanan and X. M. Lin, "Unraveling the Role of Order-to-Disorder Transition in Shear Thickening Suspensions," *Physical Review Letters* 120, 028002 (2018).



IMPACTFUL SCIENCE

#### DIAMOND NANOFEATHER STRUCTURE LAYS GROUND FOR LOW-COST FABRICATION OF ENERGY STORAGE DEVICES



Cross-sectional scanning electron microscopy image of a diamond nanofeather after an anodic etch process; small grains detach after etching, forming the feathery structure.

**THE IMPETUS** Porous diamond is an ideal material for electrical and electronic devices, such as sensors, supercapacitors, catalysts and solar energy conversion devices. However, manufacturing porous diamond is expensive. The cost of the two methods typically used, mask and etch or template and coat, vary, depending on characteristics of the material being processed. Certain properties of diamond boost the manufacturing costs: etch and growth rates of diamond are low; diamond deposition temperature is high; and diamond adhesion can be poor.

Users of the CNM from Advanced Diamond Technologies, Inc., demonstrated a new diamond nanostructure fabricated by a straightforward electrochemical etching method without masks or templates.

**THE WORK** The nanostructure is made from boron-doped nanocrystalline diamond (NCD) with a high density of grain boundaries, and it is distinct from the conventionally defined NCD or ultrananocrystalline diamond. The porous nanofeather structure has a very high aspect ratio. Preliminary characterization with Raman spectroscopy and scanning electron microscopy (SEM) indicates the fabricated diamond nanofeathers (DNFs) have a capacitance 300 times greater than the source NCD film. DNFs may well offer a third—and affordable—option for fabricating diamond nanostructures for electrical and electronic applications.

The users from Advanced Diamond Technologies, Inc., used Raman spectroscopy and high-resolution SEM resources at the CNM.

**THE IMPACT** The electrochemical etching method employed may offer a lowcost alternative to traditional diamond nano-structure fabrication techniques, eliminating masks and templates and resulting in high performance materials.

H. Zeng, N. Moldovan and G. Catausan, "Diamond Nanofeathers," *Diamond and Related Materials* 91, 165 (2019).



## **DYNAMIC LENS-ON-MEMS** BRINGS NEW VISION TO OPTICS



Optical microscope image of a lightweight, flat lens on a microelectromechanical scanner. Integration of the microelectromechanical devices with advanced flat optical surfaces will help create a new paradigm to manipulate light by combining the strength of high-speed dynamic control and precise spatial manipulation of light properties. **THE IMPETUS** Current metasurfaces are static optical elements that cannot be reconfigured after fabrication. Incorporating metasurfaces onto microelectromechanical systems (MEMS) devices creates a unique and agile lens-on-MEMS technology that paves the way for novel miniature optical systems.

A MEMS-integrated metasurface lens prototype introduces dynamic control of a new class of compact, lightweight and flat optical devices. These devices are planar counterparts of bulky optical components with the potential to reduce the size of conventional optical systems, but their static nature limits their applications. Introducing active control will greatly expand their function in optical technologies.

**THE WORK** The design involves a two-dimensional scanner micro-mirror that focuses light in the mid-infrared spectrum. When electrostatically actuated, the MEMS platform controls the angle of the lens along two axes, allowing scanning of the focal spot by about nine degrees in each direction.

The multi-diameter, disc-shaped resonators are distributed across the planar lens and separate incident and reflected beams, avoiding the need for a beam splitter. Characterization comparing mechanical response of the MEMS with and without the flat lens shows similar results, and optical focusing performance obtained experimentally confirms simulated results.

Design, fabrication and characterization were performed using optical lithography and laser capabilities at CNM and at Harvard University.

**THE IMPACT** This new dynamic metasurface lens has potential across wider fields, such as MEMS-based microscope systems and holographic and projection imaging. Designs with thousands of individually controlled devices onto a single silicon chip could lead to an unprecedented degree of control and manipulation of the optical field.

T. Roy, S. Zhang, I. W. Jung, M. Troccoli, F. Capasso and D. Lopez, "Dynamic Metasurface Lens Based on MEMS Technology," *Applied Photonics* 3, 021302 (2018).



### SOUND WAVES CARRY INFORMATION BETWEEN QUANTUM SYSTEMS



An X-ray image of sound waves (center). [Image courtesy of Kevin Satzinger and Samuel Whiteley, University of Chicago.] **THE IMPETUS** Communicating quantum information is a challenging task it is difficult to move the information more than a few microns—but, since different quantum systems represent quantum information in different ways, combining more than one type into a hybrid system could take advantage of the strengths of each one. For instance, optical photons can send quantum states across long distances, and an electron's spin state stores information, a means to expand the binary information storage system used in traditional computing. CNM researchers studied a hybrid quantum system that acoustically drives transitions in electron spin, demonstrating a basis for mechanical (strain) control of three-level spin systems.

**THE WORK** CNM researchers together with collaborators from the University of Chicago, Argonne, Tohoku University in Japan and the University of California at Santa Barbara, developed a theoretical model from a combination of direct experimental observation and density functional theory calculations, which illustrated the types of mechanical strain that drive longer-lasting spins. The researchers used silicon carbide, which has been shown recently to support long-lived spin states that can be accessed optically.

The researchers demonstrated spin transitions driven by sound waves on long-lived spin ensembles in silicon carbide through different quantum systems and compared their relative coupling strengths.

This work used the Hard X-ray Nanoprobe beamline at the CNM and Advanced Photon Source, another DOE Office of Science user facility.

**THE IMPACT** The results offer theoretical understanding and experimental demonstrations of controlling the spin states in silicon carbide. They provide a basis for quantum sensing with microelectromechanical systems (MEMS) as well as applications in electromechanical frequency filters, micro-fluidic devices and sensors in diverse areas.

S. J. Whiteley, G. Wolfowicz, C. P. Anderson, A. Bourassa, H. Ma, M. Ye, G. Koolstra, K. J. Satzinger, M. V. Holt, F. J. Heremans, A. N. Cleland, D. I. Schuster, G. Galli and D. D. Awschalom, "Spin–Phonon Interactions in Silicon Carbide Addressed by Gaussian Acoustics," *Nature Physics* 15, 490 (2019).



#### CALCITE SWITCHABLE ENCAPSULATION FOR FLEXIBLE BIO-SENSORS



Schematic of the tubular silicon nanowire field effect transistor construct with calcite as the focal encapsulation material for the sensor.

**THE IMPETUS** CNM researchers, working with CNM users and collaborators from the University of Chicago, the University of Science and Technology in China, Argonne, the University of Southampton in the United Kingdom and Hanyang University in South Korea, constructed active, flexible matrices of three-dimensional calcite that function as an array of growth regeneration sites, modeled after the specialized dynamics of fish scales. Calcite has proven itself a model system for understanding the natural process whereby living organisms produce minerals, often used for structural features like seashells and bones. Each cell in the novel active array could act as a separate growth workshop with different growth functions.

**THE WORK** This work explored applying the mineralized growth to different applications and produced three different dynamic surfaces and interfaces with separate characteristics and potential purposes. The first is a deformable surface with tunable toughness that may open new opportunities in mineral materials from synthesis to device applications. The second uses the calcite microarray to encapsulate a flexible silicon nanowire sensor. The calcite housing could enable a biocompatible sensor that can be grown in ambient conditions. The third creation established a new mechanism for underwater adhesives, in which the mineral growth serves as an inorganic localized adhesion for biological tissues or other surfaces.

Fabrication via optical and focused ion beam lithography of the field effect transistor with mutable calcite plugs occurred at the CNM. X-ray Laue diffraction and transmission X-ray microscopy measurements took place at Argonne's Advanced Photon Source, a DOE Office of Science user facility.

**THE IMPACT** The induced growth of minerals yields localized inorganic adhesion for biological tissue and dynamically reversible focal encapsulation for sensitive components such as those in flexible electronics.

J. Yi, Y. Wang, Y. Jiang, I. W. Jung, W. Liu, V. De Andrade, R. Xu, R. Parameswaran, I. R. Peters, R. Divan, X. Xiao, T. Sun, Y. Lee, W. I. Park and B. Tian, "3D Calcite Heterostructures for Dynamic and Deformable Mineralized Matrices," *Nature Communications* 8, 509 (2017).



#### SYNTHETIC PROTOCELL ENABLES SOLAR-TO-CHEMICAL ENERGY CONVERSION



Construction of a light-gated synthetic protocell. Au-Ag nanorods (green) self-assemble into the colloidal capsule (green). A light-activated protein (yellow) is fused over the surface of the capsule, creating a synthetic protocell (purple). When light shines on the protocell, the light-activated protein pumps protons through the synthetic cell membrane. At the same time, plasmonic interactions between the Au-Ag nanorods further stimulate the proton-pumping dynamics. **THE IMPETUS** Nature uses compartmentalization to achieve many different effects — particularly in structures like cells. Argonne scientists, including those from CNM, have used artificial cells to couple light harvesting to the formation of adenosine triphosphate (ATP), the unit of energy currency for biological systems. This research provides a key example of how non-biological systems can take inspiration from biology to couple light-driven processes to energy storage. Researchers anticipate that the signaling pathway between two different groups of artificial cells could be adapted for even more complex systems, like artificial neurons.

**THE WORK** The research team formed a group of colloidal capsules from an emulsion of gold and silver nanorods. These colloidal capsules formed in the presence of a purple membrane, which has the ability to pump protons when stimulated by light. The proton channel generated by the purple membrane created a proton gradient that affected a second group of artificial cells that used the protons to generate ATP.

The CNM resources used included synthesis capabilities, finite difference time domain analysis, a focused ion beam to mill and image the colloidal capsules, transmission electron microscopy, scanning electron microscopy and atomic force microscopy.

**THE IMPACT** Scientists are looking for ways to use non-biological systems that are inspired by biology in order to capture and transfer energy. In this experiment, energy harvested from light was converted into chemical energy by two distinct groups of artificial cells. The degree of cellular communication between the two groups could be refined even further.

E. A. Rozhkova, Z. Chen, G. De Queiros Silveira, X. Ma, Y. Xie, Y. Wu, E. Barry, T. Rajh, H. C. Fry and P. D. Laible, "Light Gated Synthetic Protocells for Plasmon Enhanced Chemiosmotic Gradient Generation and ATP Synthesis," *Angewandte Chemie* 131 (2019).



#### NANOCAVITY-ENHANCED OPTICAL EMISSION AT TELECOMMUNICATIONS WAVELENGTHS



Schematic of the hybrid device. Light emitted from the nanomaterial couples into, and is enhanced by, the silicon optical resonator. Inset, atomic structure of the few-layer nanomaterial. **THE IMPETUS** Silicon has been identified as a major player in the photonics industry, but it is an inefficient emitter of light. In silicon photonics, multiple discrete optical components are integrated onto a single photonic chip, but in doing so the search for silicon-based light sources has evolved from a scientific quest to solving a technological bottleneck for scalable, complementary metal-oxide-semiconductor compatible light sources. Recently, emerging two-dimensional materials have opened the prospect of tailoring material properties based on atomic layers.

**THE WORK** Few-layer phosphorene, which is isolated through exfoliation from black phosphorus (BP), is a great candidate to partner with silicon due to its layer-tunable direct band gap in the infrared where silicon is transparent. A team of CNM researchers and users from Northwestern University, Universite Paris-Sud and Thales Research and Technology, used CNM capabilities to create a hybrid silicon optical emitter composed of few-layer phosphorene nanomaterial flakes coupled to a silicon photonic crystal resonator. The research demonstrates single-mode emission near the telecommunications band of 1550 nanometers under continuous wave optical excitation at room temperature. The solution-processed few-layer BP flakes enable emission across a broad range of wavelengths.

**THE IMPACT** The research creates hundreds of hybrid silicon-based lasers in a single step, dramatically improving the prospects for silicon photonic devices.

C. Husko, J. Kang, G. Moille, J. D. Wood, Z. Han, D. Gosztola, X. Ma, S. Combrié, A. De Rossi, M. C. Hersam, X. Checoury and J. R. Guest, "Silicon-Phosphorene Nanocavity-Enhanced Optical Emission at Telecommunications Wavelengths," *Nano Letters* 18, 6515 (2018).



# THE POTENTIAL OF WAVY BOROPHENE



Atomic-resolution striped undulations in borophene on silver (111) via scanning tunneling microscopy.



Computational modeling of the strain-induced undulations.

**THE IMPETUS** The recent discovery of borophene, a two-dimensional version of boron, opened the door to a new field of boron-based nanoscale materials science. Two-dimensional materials like borophene tend to be mechanically flexible yet planar, especially when adhered on metal substrates. In borophene grown on a silver substrate, the borophene takes on a "wavy" appearance. This structure suggests that the wavy borophene would be especially stretchable.

**THE WORK** CNM researchers and collaborators combined first-principles calculations and atomic-scale ultrahigh vacuum scanning tunneling microscopy to reveal the wavy appearance of the borophene. The combination of observation and theory demonstrate that the wavy configuration is more stable than the planar form of borophene because of the anisotropic high bending flexibility of the material. The undulations are believed to be caused primarily as a source of strain relief. Borophene growth and scanning tunneling microscopy were performed by CNM scientists partnered with Northwestern University and in collaboration with the theoretical efforts led by Rice University.

**THE IMPACT** By understanding the role of strain in two-dimensional materials, scientists can design future synthesis strategies with intentional strain engineering to modify material properties. This structural model suggests the transfer of wavy borophene onto a flexible surface would allow for stretchability—with potential for flexible devices.

Z. Zhang, A. J. Mannix, Z. Hu, B. Kiraly, N. P. Guisinger, M. C. Hersam and B. I. Yakobson, "Substrate-Induced Nanoscale Undulations of Borophene on Silver," *Nano Letters* 16, 6622 (2016).



## OPTICAL "TWEEZERS" ENABLE ANALYSIS OF CRYSTALS IN LIQUIDS



Depiction of "optical tweezers" using lasers, a mirror and a light modulator to anchor a crystal in solution, making it possible to conduct X-ray diffraction measurements.

**THE IMPETUS** Optical trapping is a known noncontact sample manipulation technique to study the structure and dynamics of nano- and mesoscale objects without inducing undesired changes in structure. Combining optical trapping with hard X-ray microscopy techniques, such as coherent diffraction imaging and crystallography, provides a nonperturbing environment where electronic and structural dynamics of an individual particle in solution can be followed in situ. A team of CNM researchers together with users and collaborators from Argonne, Brookhaven National Laboratory, the University of Chicago, Clarkson University and the University of Maryland, demonstrate that dynamic holographic optical tweezers are capable of manipulating single micrometerscale anisotropic particles in a microfluidic environment with the precision and stability required for X-ray Bragg diffraction experiments—thus functioning as an "optical goniometer."

**THE WORK** This work demonstrates that dynamic holographic optical tweezers are capable of manipulating single micrometer-scale anisotropic particles in a fluid environment with the precision and stability required for synchrotron X-ray diffraction experiments. This noncontact sample manipulation technique of optical trapping allows for manipulating single particles in solution, without inducing undesired changes in structure, to obtain three-dimensional maps of shape and strain.

Microfluidic cell fabrication and electrodynamics simulations were performed on Carbon, CNM's high performance computing cluster. X-ray diffraction data were collected at beamline 34-ID-C at Argonne's Advanced Photon Source, a DOE Office of Science user facility. This method, based on dynamic holographic optical trapping in a standing-wave geometry, allows sufficient angular stability to perform Bragg coherent X-ray diffraction imaging.

**THE IMPACT** Obtaining a fundamental understanding of crystal growth and chemical reactions in solution is of broad interest for materials discovery, structural biology and catalysis.

Y. Gao, R. Harder, S. H. Southworth, J. R. Guest, X. Huang, Z. Yan, L. E. Ocola, Y. Yifat, N. Sule, P. J. Ho, M. Pelton, N. F. Scherer and L. Young, "Three-Dimensional Optical Trapping and Orientation of Microparticles for Coherent X-ray Diffraction Imaging," *Proceedings of the National Academy of Sciences of the United States of America* 116 (10), 4018–4024 (2019).

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