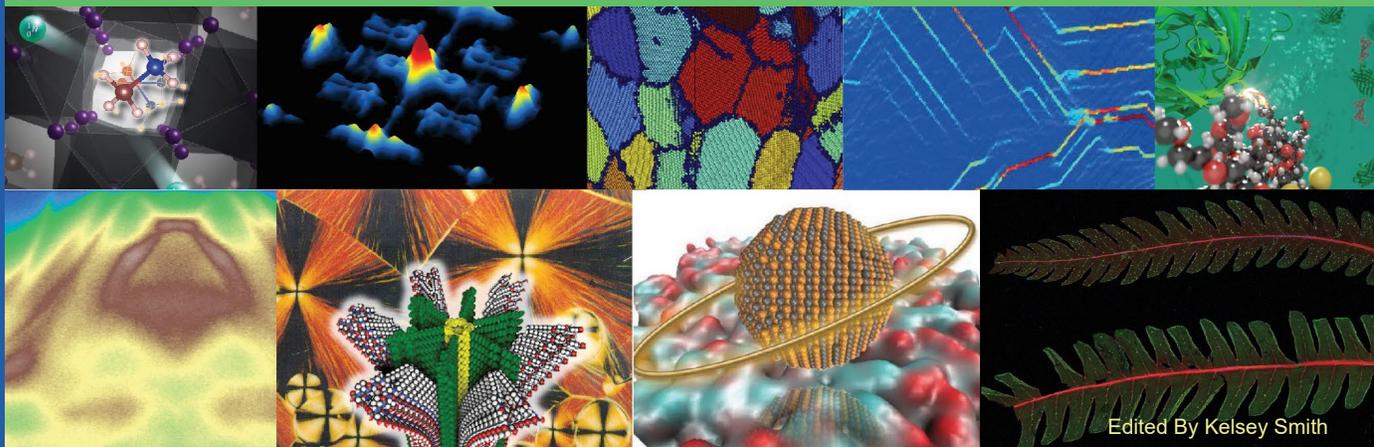




VOLUME 2  
ISSUE 1

# DMR DIVISION OF MATERIALS RESEARCH

## DIRECTORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES



Edited By Kelsey Smith

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## Did You Know?

### We've Moved!

The National Science Foundation's (NSF) headquarters are now located at 2415 Eisenhower Avenue in Alexandria, Virginia.

### We Have a New Solicitation

We have a new Topical Materials Research Programs (TMRP) solicitation for six of the eight Division of Materials Research programs. For more information, please visit the [TMRP solicitation](#) or check out our TMRP update on [page 6](#) for more information.

### Revised Proposal & Award Policies & Procedures Guide (PAPPG)

A revised version of the NSF's PAPPG has been issued. The new PAPPG is effective for proposals submitted, or due, on or after January 29, 2018. Please check out the revised [PAPPG](#) for any changes.

### New Research.gov Proposal Preparation

As of April 30, 2018, proposers are able to prepare and submit full, research non-collaborative proposals in Research.gov. The initial release of this new Research.gov capability runs in parallel with existing FastLane proposal preparation and submission capabilities, so proposers can choose to prepare and submit full, research non-collaborative proposals in Research.gov or in FastLane as of April 30, 2018. Test it out [here!](#)

### Need Helium? The APS Has a New Plan!

APS, in partnership with MRS and ACS, recently launched a [website](#) that connects researchers who rely on helium with companies that can help them transition to helium-conserving technologies. The [website](#) helps researchers determine if it is economically favorable to transition to equipment that reduces helium usage and provides the option to be contacted directly by equipment vendors. DMR provides funding for liquid helium needs and equipment recycling needs. Please contact your Program Director for more information.

## No Summer Break for DMR

The peak of cherry blossom season in Washington D.C. has come and gone, but the summer weather is just arriving. Summer is an extremely busy time for the National Science Foundation (NSF) and the Division of Materials Research (DMR). Budgets and strategic planning have been heavy on our minds.

However, DMR was proud to have recently renewed the internationally leading, NSF-funded [National High Magnetic Field Laboratory \(NHMFL\)](#) that has produced three world record-breaking, high-field magnets in less than two years. These technological advances will enable important experiments for researchers to discover new physics, chemistry, and biology related to quantum materials, chemical dark matter, and structure, function, and regulation. DMR is also gratified in promoting a multi-year process to transition NSF's stewardship of the Cornell High Energy Synchrotron Source (CHESS) to a partnership model. A CHESS upgrade, [CHESS-U](#), supported by the State of New York, should be completed this year, resulting in a premier synchrotron source in the U.S. for high-energy, high-flux X-ray studies. This upgrade will enable new scientific capabilities at CHESS, including enhanced microspectroscopy for a variety of life sciences, improved time-resolved X-ray diffraction for both metallurgical metals/alloys, as well as fundamental studies into strongly correlated materials. DMR also supports the sub-facility, Center for High Resolution Neutron Scattering (CHRNS) at the National Institute of Standards and Technology Center for Neutron Research, which will be evaluated next year for renewal. You will read about these major facilities in this newsletter, along with other DMR-supported facilities and instrumentation available to researchers, including the Materials Research Facilities Network (MRFN), an excellent example of instrumentation made available to you to advance your research and collaborations; and the National Nano-Coordinated Infrastructure (NNCI, formerly known as the NNIN). In this partnership with the Engineering Directorate, DMR makes available nanofabrication and testing instrumentation to the materials research community. I strongly encourage you to read about gaining access to these resources on [pages 7 – 10](#).

We also update you on our efforts to help build a data infrastructure for the materials research

community, necessary for realizing the vision of the Materials Genome Initiative (MGI). While Designing Materials to Revolutionize and Engineer our Future program, NSF's main response to MGI is not being offered in 2018, DMR was active with the Principal Investigators of this program in building data capabilities. [Page 4](#) describes how the two Materials Innovation Platforms, 2DCC and PARADIM, are leading an effort to connect researchers together through data generated on 2D materials.

In 2016, DMR partnered with the Department of Energy/Basic Energy Sciences to sponsor the National Academies to conduct a decadal study of materials research. Many of you may have contributed to numerous town halls held over the last 18 months regarding this study. We are anticipating the study to be completed this summer and published in the fall. Coinciding with this study, DMR has been busy internally developing a divisional strategic plan. This is partly in response to our [2015 Committee of Visitors \(COV\) report](#), noting "The historical impact of DMR-funded research is impressive, but the COV judged that there is an urgent need to benchmark the investment in basic materials research in DMR in a global context." Our next COV meeting will take place in September 2019, where we will present the DMR Strategic Plan and receive valuable feedback from the materials research community.

Until then, all DMR staff will be working hard to review and make recommendations on the materials research proposals submitted this year through our new [Topical Materials Research Program solicitation](#). DMR thanks all of you for your valuable time and partnership with us to promote the progress of science for the good of the Nation.

*Linda S. Sapochak*  
Division Director of DMR



## DMR's Presence at the APS March Meeting 2018

At the American Physical Society (APS) March 2018 Meeting in Los Angeles, the DMR ran a special session on Monday evening, entitled "[Enabling Quantum Leap: Federal and Private Funding Opportunities in Condensed Matter Physics and Materials Science](#)." This well-attended session outlined the funding opportunities at the National Science Foundation (NSF), the Department of Energy, the Air Force Office of Scientific Research, the Gordon and Betty Moore Foundation, and the Army Research Office available to Principal Investigators (PIs) in the area of Condensed Matter Physics and Materials Science. DMR held a speed-coaching event on Tuesday and Wednesday, titled "Meet Your Program Director." Interested active and potential PIs and students could sign-up at the NSF booth in the Exhibit Hall in the morning for a 15-minute, one-on-one meeting with a Program Director of their choice in the afternoon. Over the two-day period DMR spoke with over 120 PIs, hearing about excellent research ideas, providing advice on

proposal submissions, and answering questions related to the NSF process. Additional activity at the APS 2018 meeting included a well-attended session that discussed DMR's Polymer program and highlighted the most recent Polymer Decadal Workshop, as well as answered questions from the audience. For more information on the Polymer Decadal Workshop, please check out our "[Frontiers in Polymer Science and Engineering](#)" article.



**Figure 1.** DMR Program Directors meet with Principal Investigators during the "Meet Your Program Director" event at the APS March Meeting 2018. Image courtesy of Tomasz Durakiewicz.

## Young Investigator Workshop



**Figure 2.** Early career investigators attending the Young Investigator Workshop on June 8 - 9, 2017. Image courtesy of Paul Sokol.

DMR held the Young Investigator Workshop on June 8 - 9, 2017. Roughly 70 young faculty from 50 different universities attended the workshop, making it the largest to date. The Young Investigator Workshop aims to provide faculty at the beginning of their careers with information on the funding opportunities for materials research within DMR and advice on how to write successful proposals to NSF. Dr. Linda Sapochak, DMR's Division Director, began the workshop with an overview presentation of DMR's programs and goals. Several talks by program officers provided details on the various funding opportunities available to young faculty, such as the Topical Materials Research Programs (TMRP) and CAREER programs, international funding

opportunities, and other multi-investor opportunities within DMR. Other sessions provided advice on how to write successful proposals and understanding the review process. Several senior faculty also provided their wisdom on how to survive and thrive as a junior faculty member (Dr. Iannacchione, Worcester Polytechnic Institute), broadening participation (Dr. Hodapp, American Physical Society), and communicating with the public (Dr. Adenwalla, University of Nebraska). Dr. Hamlin (University of Florida) provided a helpful talk on mistakes to not make as a young Principal Investigator. A popular component of the workshop, "Dinner with a Program Officer," allowed young faculty and program officers to become better acquainted in an informal setting. This workshop provides early career investigators with the information they will need to be successful. Several alumni of a similar workshop held by the Condensed Matter Physics (CMP) program, credited this workshop with helping them be successful in their endeavors.

# Empowering the Materials Research Community to Harness Data

Eva Campo and Alex Klironomos

NSF has recently unveiled an innovative vision strategy through the conception of 10 Big Ideas that will inspire, promote, and advance key developments fostering cutting-edge global science and engineering leadership. The Harnessing the Data Revolution (HDR) Big Idea represents a thrust to transform research through new insights gained from data. HDR is particularly relevant for the community supported by DMR.

In response, DMR has recently created the Data Working Group (DMR-DWG). The purpose of the group is to empower the materials research community to embrace data in a diverse fashion. Anticipated challenges throughout HDR in materials research include the need to develop and adopt data-friendly research practices, to develop data infrastructure, to facilitate training, to develop the work-force and community, as well as to foster progressively deeper interactions with computer and



**Figure 4.** The audience at Penn State listening to the DMR-2D Data Framework session. Image courtesy of Penn State.

Innovation Platforms (MIP), Designing Materials to Revolutionize and Engineer Our Future (DMREF), Partnerships for Research and Education in Materials (PREM), and Emerging Frontiers in Research and Innovation (EFRI) grantees. During the workshop, PIs from diverse backgrounds provided a wealth of feedback that articulated a vision of a dynamic, structured, and well-networked

**“PIs provided a wealth of feedback that articulated a vision of a dynamic, structured, and well-networked community working on 2D materials: the DMR-2D Data Framework.”**

data scientists.

Taking a first step towards orchestrating a response, the DMR-DWG designed and organized a highly interactive, community-led brainstorming session during a grantees meeting at Penn State in November 2017, involving Materials



**Figure 3.** A PI presenting a white paper pitch featuring a collaboration between EFRI and MIP. Image courtesy of Penn State.

community working on 2D materials: the DMR-2D Data Framework.

Additionally, white papers were solicited from the community. Through competition and as identified by the scientific community, the most compelling and urgent data-centric projects were funded. This bottom-up approach has identified the MIPs as the center of the DMR-2D Data Framework, and the first near-neighbor positions are currently being populated by materials researchers with demonstrated data expertise. These influencers will help link materials scientists with resources to further enable data-intensive research. The DMR-DWG is working to deploy similar approaches in other topical areas, seeking to further enable the capabilities of the materials research community to harness data.

## Need a New Graduate Student? Try AGEP-GRS and MPS-GRSV!

Anne Kornahrens

The Alliances for Graduate Education and the Professoriate (AGEP) program from the Directorate for Education and Human Resources (EHR) supports historically underrepresented minority (URM) faculty in Science, Technology, Engineering, and Mathematics (STEM) and Education research fields. After multiple evolutions, AGEP awardees now aim to advance knowledge about models to improve pathways to the professoriate and success for historically URM doctoral students, postdoctoral fellows and faculty. The Directorate for Mathematical and Physical Science (MPS) AGEP-Graduate Research Supplements (AGEP-GRS) opportunity is designed to allow MPS-supported researchers to bring on a new graduate student into their research group to engage in broadening participation of URMs. The MPS-specific offering was first announced through a Dear Colleague Letter (DCL) in 2012 and has supported 160 students thus far in DMR. The MPS AGEP-GRS supplements allow a PI of a currently active MPS research award to apply for a supplement to cover tuition and stipend support for a new graduate student. The initial 12 months of support typically ranges from \$45-60K, and can be renewed for up to three years. In 2013, the AGEP-GRS institutional eligibility expanded to include AGEP Legacy schools, rather than limiting it to currently active AGEP academic units.

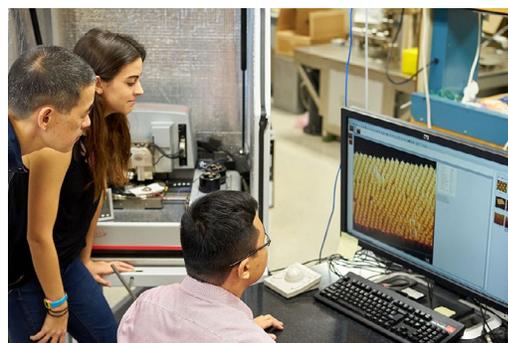
A subsequent DCL in 2015 expanded this supplement opportunity to full-time veteran STEM Ph.D. students at any school through the MPS-Graduate Research Supplement for Veterans (MPS-GRSV). For more information, see the DCLs ([AGEP-GRS DCL](#) and [MPS-GRSV DCL](#)) and contact your DMR Program Director or Dr. Kornahrens ([ankornah@nsf.gov](mailto:ankornah@nsf.gov)) at NSF to discuss this opportunity.

## New MRSEC Centers, New Discoveries

**Eight DMR center awards were given in 2017; three are new Materials Research Science and Engineering Centers (MRSECs) and the five remaining were renewal MRSECs.**

There are currently a total of 20 MRSECs funded by the National Science Foundation. These MRSEC centers cover all areas of materials science and help encourage collaborations regionally, nationally, and internationally. These six-year MRSEC awards are a significant investment in materials science and will have future impacts on multiple fields of research.

The three new MRSECs were awarded to the University of Texas-Austin, the University of Illinois at Urbana-Champaign, and the University of Washington. The Center for Dynamics and Control of Materials, the new MRSEC at the University of Texas-Austin, seeks to encompass the understanding and control of materials over extended temporal and spatial scales. The University of Illinois at Urbana-Champaign's new MRSEC seeks to understand the dynamic properties of materials. The Molecular Engineering Materials Center (MEM-C), the new MRSEC at the University of Washington, seeks to utilize team-based development of novel electronic and photonic materials that are relevant to future high-tech applications. For more information on the five MRSEC center renewals, please visit the [MRSEC website](#). These MRSEC centers will provide leadership for the country concerning new materials and new materials phenomena. More information about the MRSEC program can be found [here](#).



**Figure 5.** Cockrell School of Engineering professor and new Center for Dynamics and Control of Materials director Edward Yu (left) with undergraduate student Cassandra Huff and graduate student Zhongjian Zhang. Image courtesy of the University of Texas-Austin.



## Access to Infrastructure

Leonard Spinu, Guebre Tessema, Charles Ying, and Dan Finotello

The complexity of modern materials research is such that new advances in the field depend on the research community having access to a broad range of tools, of different scales such as those found at large facilities, medium scale facilities, interdisciplinary research centers, and individual investigators' laboratories. The Division of Materials Research supports access to large national facilities, as well as to medium scale platforms.

DMR's National Facilities and Instrumentation (NaFI) program provides the Nation's universities and colleges access to cutting edge tools for research and training in materials research and related fields. NaFI's current portfolio is the result of a history of engaging the community in identifying critical needs for tools to advance the frontiers of materials research. Its portfolio reflects the cooperative stewardship model for managing the Nation's major facilities and includes stewardship of unique large facilities, as well as partnership with other federal agencies. Management of the national facilities is following either a stewardship or partnership model, i.e., a shared management with partners from NSF and other federal agencies.

The DMR national facilities are uniquely large multi-user facilities requiring a budget level that is not readily affordable by one university or state. DMR is the steward for these national facilities, which include, for example, the National High Magnetic Field Laboratory and the Cornell High Energy Synchrotron Source.

## National High Magnetic Field Laboratory (NHMFL)

### NATIONAL HIGH MAGNETIC FIELD LABORATORY



#### Mission

- Provide the U.S. colleges and universities with the highest magnetic fields and necessary services for scientific research in a wide range of disciplines
- Train the next generation of scientists in magnet science and technology

#### Highlights

- The largest and highest-powered magnet laboratory in the world
- Provides access to more than 1,700 users annually
- Record for highest field for a continuous field magnet (45 Tesla) and highest controlled wave milliseconds pulsed field (100 Tesla)

#### Capabilities

- Seven user facilities across three sites
- Includes DC Field, Pulsed Field, Advanced Magnetic Resonance Imaging and Spectroscopy, Electron Magnetic Resonance, High B/T, Ion Cyclotron Resonance, Nuclear Magnetic Resonance and Magnetic Resonance Imaging

#### Locations

- Florida State University, Tallahassee, Florida (top)
- Los Alamos, New Mexico (center)
- University of Florida, Gainesville, Florida (bottom)

#### User Access

Open user access to scientists around the world, free-of-charge, based on a competitive proposal process. All user facilities accept proposals throughout the year. For more information, please visit [NHMFL's website](#).

# Cornell High Energy Synchrotron Source (CHESS)

## Mission

- Provide a national hard X-ray synchrotron radiation facility
- Provide research and development of new synchrotron radiation technologies and upgrading of the facility
- Provide integration of research and education into the training of personnel
- Provide educational outreach to expose K-12 students and the public to synchrotron X-ray science and its application to materials research

## Capabilities

- One of only two hard X-ray sources in the U.S.
- Operates 11 beamlines for structural and spectroscopic studies of materials and biological systems



## Highlights

- Grown its user community
- Provides access to more than 1,000 unique users annually
- 20% of users are from abroad
- Two of its users over the last 30 years have received the Nobel Prize
- Many trainees have gone on to lead or operate major synchrotron facilities worldwide

## Location

- Cornell University, Ithaca, New York



## User Access

Open user access available free-of-charge to all scientists and engineers from around the world. Users have access to a wide variety of unique experimental stations based on a competitive proposal review process. For more information, please visit [CHESS' website](#).

# Center for High Energy Neutron Scattering (CHRNS)



## Mission

- Enable access to specialized world class neutron instruments to researchers in broad areas of science including quantum hard matter, soft condensed matter, biology, polymers, and rheology of complex fluids
- Develop neutron scattering expertise in the U.S.

## Capabilities

- Operates five neutron scattering instruments
- Includes a 30-meter, high resolution, small-angle neutron scattering instrument; a diffractometer for ultra-high-resolution small-angle scattering; a multi-axis crystal spectrometer; a backscattering spectrometer with 1  $\mu\text{eV}$  resolution; and a neutron spin echo spectrometer

## Highlights

- Offers roughly 1,000 instrument days per year with 99% reliability
- Specialized summer school on neutron scattering hosts roughly 30-36 students per year

## Location

- NIST Center for Neutron Research, Gaithersburg, Maryland

## User Access

CHRNS offers the use of neutron scattering instrumentation open and free-of-charge to all qualified users based on peer-reviewed proposals. Calls for proposals are issued every six to seven months. For more information, please visit [CHRNS' website](#).

# ChemMatCARS

## Mission

- Develop and operate world-class synchrotron X-ray facilities serving the needs of users in chemistry and materials research
- Funded by NSF's Divisions of Chemistry and Materials Research
- National user facility for frontier research in chemistry and materials science using synchrotron x-rays at the Advanced Photon Source (APS)

## Location

- Argonne National Laboratory, Argonne, Illinois

## Capabilities

- Operates three experimental stations in the areas of advanced small-molecule crystallography, liquid surface and interface scattering, and small to wide-angle scattering at the APS

## Highlights

- Provides access to roughly 1,000 users
- Annual Neutron X-Ray School on Liquid Surface and Scattering allow students to determine the structure and ordering of the Langmuir monolayer of phospholipid molecules

## User Access

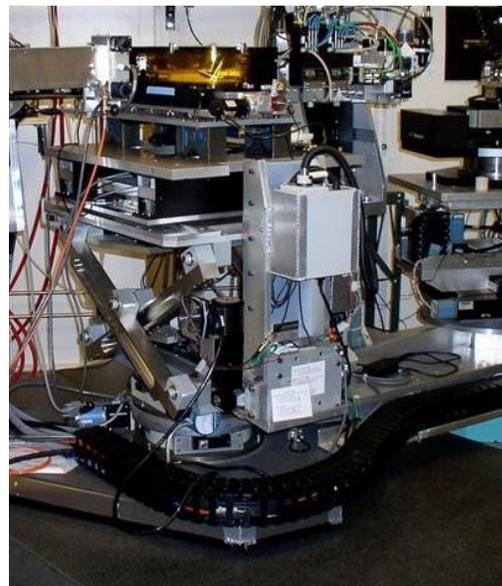
Open user access available free-of-charge to all scientists from around the world. All users of the ChemMatCARS beamline must apply for beamtime by submitting a proposal to the APS General User Program by the appropriate APS Deadline. For more information, please visit [ChemMatCARS' website](#).



THE UNIVERSITY OF  
CHICAGO



Main Steward: NSF's Division of  
Chemistry



# National Nanotechnology Coordinated Infrastructure (NNCI)



Main Steward: NSF's Division of  
Electrical, Communications and  
Cyber Systems



## Mission

- Advance research in nanoscale science, engineering, and technology
- Enable greater national impact of nanotech innovation and commercialization
- Co-funded by NSF's Divisions of Chemistry and Materials Research, and Directorates for Biological Sciences and Engineering

## Highlights

- Provides access to roughly 11,000 users
- Includes more than 2,500 external users
- Represents 200 academic institutions and roughly 700 companies

## Capabilities

- Offers access to more than 2,000 leading-edge fabrication and characterization tools, instrumentation, and expertise within all disciplines of nanoscale science, engineering and technology
- Sponsors "Science Outside the Lab" which gives graduate student scientists and engineers a glimpse at how the government shapes science

## Location

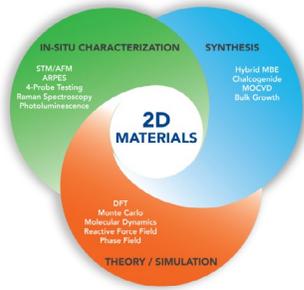
- Comprised of a network of 16 institutions spread around the continental USA and a coordinating office at Georgia Tech

## User Access

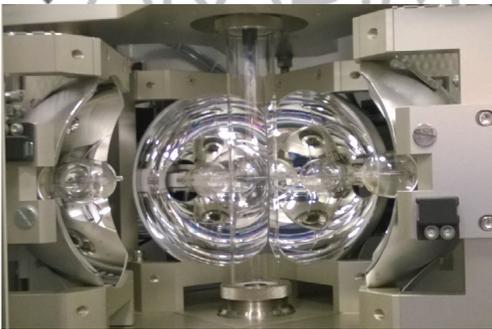
NNCI sites are established as independent operating units by the NSF. Each site has developed its own procedures for new user access and applicable fees, and you can find those on each of the individual site pages. For more information, please visit [NNCI's website](#).

# Materials Innovation Platforms (MIP)

## 2D Crystal Consortium NSF Materials Innovation Platform



PARADIM



### Mission

- Devoted to accelerating the discovery of new materials in a focused science area
- Serve as a user facility
- Provide access to a broad range of instrument and computational capabilities as well as expert samples

### Capabilities

- Offer comprehensive thin-film growth equipment including molecular beam epitaxy with in-situ angle-resolved photo emission spectroscopy and chemical vapor deposition and bulk crystal growth
- Offer theory and simulation support related to 2D materials synthesis related to growth kinetics and characterization

### Highlights

- Offered an Electron Microscopy Workshop and a Graphene and Beyond Workshop with 2DCC
- Advanced future generation electronics with 2D materials
- Developed a fast non-destructive test for 2D materials

### Locations

- Cornell University and Johns Hopkins University
- Pennsylvania State University and Clark Atlanta University

### User Access

MIPs accept user proposals year-round with no user fee from scientists interested in the synthesis of 2D materials. The proposals can be for user access of the fabrication facilities, sample request and/or theory and simulation consulting. For more information, please visit [PARADIM's website](#) and the [2D Crystal Consortium \(2DCC\) at Penn State's website](#).

# Materials Research Facilities Network (MRFN)

### Mission

- Nationwide partnership of the Shared Experimental Facilities (SEFs)
- Designed and operated to provide support to researchers and experimental facilities engaged in the broad area of Materials Research in academic, government, and industrial laboratories around the world
- Provide information on the latest experimental and theoretical techniques with more than 200 experts

### Capabilities

- Includes 1,137 instruments in the wide range of materials synthesis, fabrication, and characterization distributed at the 20 MRSECs and with the support of 262 experts

### Highlights

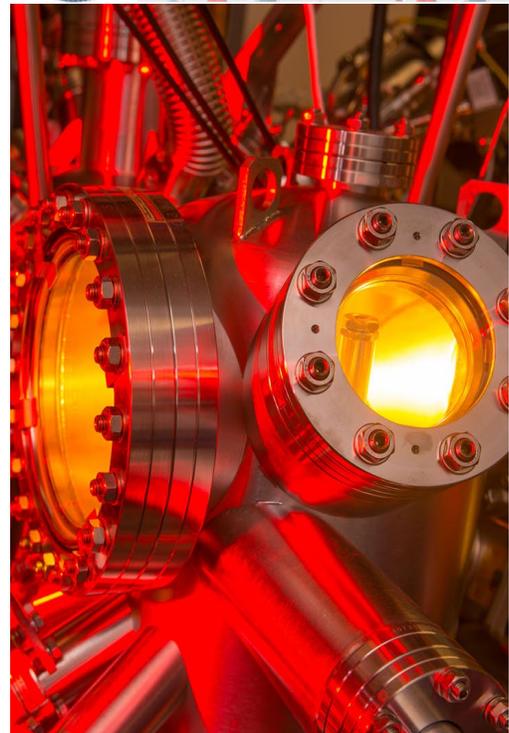
- Boasts 20 participating MRSECs
- Functions as a nationwide robust network to promote and support the growth of the materials science field in the U.S.
- More than 2,000 researchers use MRFN equipment and expertise

### Location

- 20 NSF-funded MRSECs across the U.S.

### User Access

Users have access to a wide variety of unique experimental stations based on a competitive proposal review process. Prices vary based on hours, use, session, and type of equipment. For more information, please visit [MRFN's website](#).



# My Life as a Rotator

Paul Sokol



**Figure 7.** Paul Sokol, former Program Director for the Condensed Matter Physics Program (CMP) in DMR.

My time serving as a program director (PD) for the Condensed Matter Physics (CMP) program at the National Science Foundation (NSF) was an intense learning experience that I enjoyed immensely.

The rotator program at the NSF primarily brings in academic scientists from outside the Foundation as

temporary PDs. These rotators trade in their academic responsibilities of teaching, research, and service, for the job of getting proposals reviewed and making funding recommendations based on those reviews. This program gives rotators a broader view of their community, as well as a behind-the-scenes view of “how it’s made.” In return, NSF receives an infusion of fresh ideas and an important connection to the academic community it funds.

The CMP program, the largest DMR program funding individual investigators, has a broad portfolio ranging from superconductivity and magnetism to colloids and quantum fluids. As a PD for a brief time period, I was given the opportunity to learn about all of these areas, both from the proposals NSF received and from the review panels that discussed them.

PDs have an extremely important role at NSF and are responsible for making funding recommendations, which are ultimately approved by the Division Director. This sets the scientific direction in the CMP-funded fields and can greatly impact the faculty seeking funding. Thankfully, NSF receives help with this process from the community’s reviews and participation in panels. However, the job of the PD is not that of a simple bookkeeper, whose sole responsibility is counting up the “Excellent” and “Very Good” ratings and giving money to whoever has the highest marks. The PD also has to consider how the funding

recommendation will affect the health of the field. Examples of these additional factors include:

## Additional Factors to Consider

- Have new and controversial ideas received a fair hearing?
- Is NSF funding enough assistant professors?
- Is NSF supporting diversity in our principal investigators?
- Is NSF ensuring a robust community at all sorts of different institutions?

Making funding recommendations is never easy. It is impossible to fund all of the good proposals that CMP receives every year; however providing advice to PIs on improving their proposal and seeing it succeed on resubmission is equally rewarding.

I was surprised by the freedom that the NSF offered its rotators beyond just managing their programs. For example, after expressing concern about the success of young PIs, DMR funded a successful workshop for young investigators that gave them advice on writing successful proposals and introduced them to the NSF programs. After originating in the CMP program, this workshop has now become an annual event that encompasses all of DMR. Additionally, I was given the opportunity to work with the National Academies on several projects such as participating in condensed matter physics panels, participating in international unions, and beginning the current decadal survey of materials research.

One of the most rewarding parts of serving as a rotator was the people I had the opportunity to work with at DMR. The other PDs and the administrative staff were always willing to help and everyone worked toward funding the best possible science. I can say without doubt that the job would have been impossible without the support of the DMR staff. I truly enjoyed working with DMR and value the friendships I developed while there. While I’m glad to return to the university life, I am happy for the opportunity to have worked as a rotator and I left the NSF with a sense of accomplishment.

# QS<sup>3</sup>: Enabling the Quantum Leap

Tomasz Durakiewicz

Representatives of industry, funding agencies, and research communities have identified the painful problem of the missing pipeline that would enable the second quantum revolution: the United States is currently not educating students in sufficient numbers with knowledge, understanding, and expertise in multiple convergent fields. The Quantum Science Summer School (QS<sup>3</sup>) is leveraging the existing expertise in quantum technologies and the years of the National Science Foundation's investments that have built and nurture this expertise, to equip a large contingent of talented students with cutting-edge knowledge and hands-on experience required by the second quantum revolution.

QS<sup>3</sup>, funded jointly by NSF and the Department of Energy (DOE), offers a view of the future quantum



**Figure 9.** “A Crash Course in Machine Learning,” an interactive session run by Google. Image courtesy of Linda Ye and Joe Checkelsky.

Materials and Devices. A combination of morning talks and afternoon interactive events helps forge the “transdisciplinary student,” who fulfills the needs of the quantum revolution, with connections to both research and that industry. The student selection

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**“The future quantum worker is a product of a ‘quantum superposition’ of convergent science disciplines.”**

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worker as a product of a “quantum superposition” of science disciplines of Materials and Chemistry, Engineering, Physics, and Computer Sciences. Each of the four consecutive annual Schools span two weeks and include about 50 students exposed to a training profile covering convergent disciplines. These Schools include speakers from industry and researchers representing Quantum Computing, Engineering, Cold Atom Physics, Chemistry, Social Sciences, National Facilities, and Quantum

$$\begin{aligned} |\text{Quantum Scientist}\rangle = & C_1 |\text{Materials \& Chemistry}\rangle + C_2 |\text{Engineering}\rangle \\ & + C_3 |\text{Physics}\rangle + C_4 |\text{Computer Science}\rangle \end{aligned}$$

**Figure 8.** Education of a “Quantum Scientist” requires training in materials, chemistry, engineering, physics, and computer science disciplines. In the spirit of QS<sup>3</sup>, a quantum scientist is a “superposition” of experts in these convergent fields. Image courtesy of Linda Ye and Joe Checkelsky.

process ensures a diverse student population from varied and highly interdisciplinary backgrounds are selected.

The first QS<sup>3</sup>, focused on Quantum Information, was organized at Johns Hopkins University from June 5 – 16, 2017. A total of 69 participants attended, with 16 lecturers, five organizers, and 48 graduate students. A quarter of the participants in that first QS<sup>3</sup> were female. Industry lecturers included participants from IBM, Google, Lincoln Laboratory, and the Los Alamos National Laboratory. Over 200 graduate applicants expressed interest in the first QS<sup>3</sup>, demonstrating the need and interest in this useful and fun event. The next edition of QS<sup>3</sup> will focus on Quantum Materials and is currently planned for June 11 – 22, 2018, at Cornell University. Subsequent QS<sup>3</sup> Schools will be held at Pennsylvania State University in 2019 and the University of Colorado in 2020. Please visit the QS<sup>3</sup> School's [website](#) for more information.

# Frontiers in Polymer Science and Engineering

Andrew Lovinger

The report for the National Science Foundation's (NSF) third decadal study workshop concerning the field of polymer science and engineering, held in August 2016, has been issued. Two previous decadal studies were held in 1997 and 2007. The [Frontiers in Polymer Science and Engineering](#) workshop report, co-sponsored by a number of federal agencies (AFRL/AFOSR, ARO, DOE/BES, FDA, NIST, and ONR) and other NSF Divisions (CBET, CHE, and CMMI), focused on the following themes:

## Frontiers in Polymer Science and Engineering Report Themes

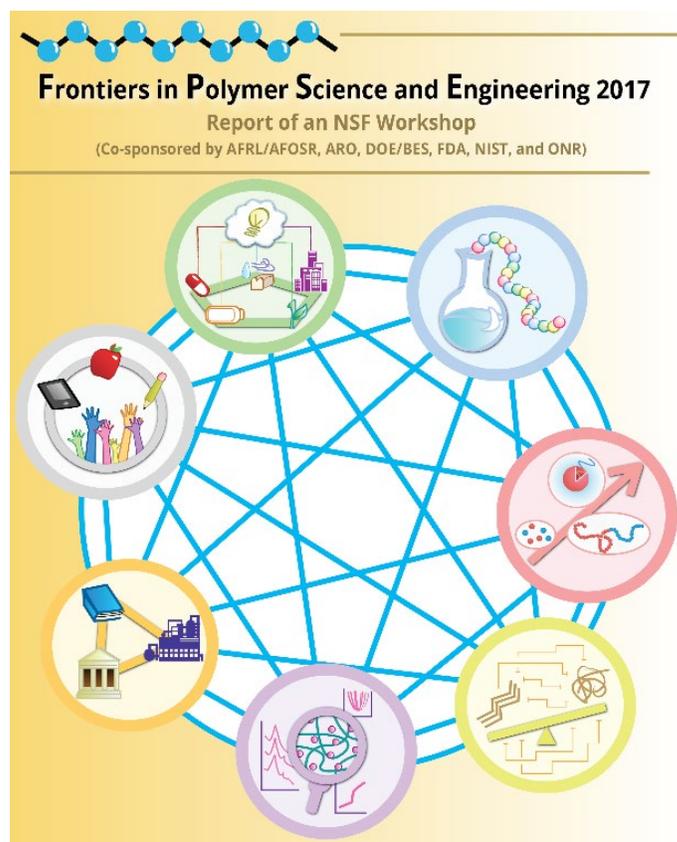
- Societal Needs and Impact
- Macromolecular Synthesis
- Hierarchical Structures at Multiple Length and Energy Scales
- Integrated Measurement, Analysis, and Prediction
- Advancing Performance
- Partnerships: Academia, Industry, and Government
- Higher Education and Diversity
- Outreach and Broadening Participation

The workshop, attended by more than 100 participants from academia, industry, national laboratories, foreign institutions, and the federal government, was organized by a steering committee chaired by Dr. Frank Bates (University of Minnesota). Members of the steering committee included Dr. Patrick Brant (ExxonMobil), Dr. Geoffrey Coates (Cornell University), Dr. Juan de Pablo (University of Chicago), Dr. Jane Lipson (Dartmouth College), Dr. Chinedum Osuji (Yale University), Dr. Stuart Rowan (Case Western Reserve University, now at University of Chicago), Dr. Rachel Segalman (University of California Santa Barbara), and Dr. Karen Winey (University of Pennsylvania). Their excellent organization of this third decadal study was instrumental in the resulting report.

The findings and recommendations of the workshop were presented during the 2017 American Chemical

Society's joint award session of the Polymeric Materials Science and Engineering Division (PMSE) and the Polymer Chemistry Divisions (POLY) plenary lecture by Dr. Bates.

Further coverage of the report and its recommendations can be found in the September 2017 issue of the Materials Research Society Bulletin. The article, titled "[Third NSF Decadal Report Presents Challenges for Polymer Field](#)," describes the report as "notable because it spans the entire field of polymer science and engineering," and ultimately concludes that the report "admirably summarizes the pervasiveness, importance, and economic impact of polymers." A [Physics Today](#) article comments on the instrumental nature of polymers on solving society's problems, but cautions that creating a sustainable polymer industry that encourages appropriate disposal of plastic materials is a "daunting challenge" that has yet to be solved.



**Figure 10.** The Frontiers in Polymer Science and Engineering 2017 Report is available [here](#).

# Materials Solutions Begin with Data

Daryl Hess

Imagine using a neural network to solve Schrödinger's equation at a fraction of the current computation cost. Imagine using currently available data to pinpoint the next costly experiment that most illuminates the landscape of a complex phase diagram. These possibilities, and more, rest on Finding, Accessing, Interoperating, and Reusing (FAIR) digital data. Implementing FAIR data solutions for materials data enables the materials research community to build on the works of others more effectively, rapidly, and in parallel fashions to accelerate the scientific process. Exploring the possibilities and achieving the potential of data-centric and data-intensive research at all levels from individual investigators, to teams, to centers and to facilities, requires the effective use of data analytics and a data infrastructure.

Creation of a high performance and useful data infrastructure is a collaborative interdisciplinary effort that includes the active engagement of materials researchers, cyberinfrastructure experts, and computer scientists. The infrastructure will involve hardware, software cybertools, and ultimately the people that will create and use an infrastructure that can foster a culture of data-sharing and data-on-demand. They will harness the opportunity presented by the “big data revolution” and will pave the way for data-driven research to become an effective tool to conduct meaningful science.

Success requires the ability to share and access data from experiments and diverse computational research of all kinds. Novel hardware and software to automate critical aspects of materials data science, such as curation, preprocessing, dissemination, and consistency checking, right at the instrument or instruments of data origin, may provide a valuable mechanism to reduce the overhead of the transformation to a data-sharing materials research community. Clever and innovative incorporation of data-intensive approaches into the synergistic interaction loop of theory/computation and experiment plays a critical role in realizing new materials products in half the time and at a fraction of the cost.

Creatively developing data cyberinfrastructure lies outside the scope of support of most programs, but Cyberinfrastructure for Sustained Scientific Innovation (CSSI) can support the envisioned interdisciplinary collaborations to unleash a new dimension of innovation in science. The [Local Spectroscopy Data Infrastructure \(LSDI\)](#) provides an example of this vision. Viewed from afar, the route to develop an effective data infrastructure seems far from certain. However, a sensible strategy might maximize science driving the creation of data infrastructure. This can ensure that progress made survives beyond challenges of funding and rapidly evolving technologies.

These strategies driven by science can build the outposts at the materials data frontiers where innovation is welcome to make the next leap of progress; outposts that lay the foundations for future data cyberinfrastructure nodes that are well tailored to the needs and culture of the materials research community. Combining data-intensive methods with computation, experiment, and theoretical advances might be the solution to energize materials research and unleash a creativity that better discovers new materials, new states of matter, and new phenomena, and enables the solution of critical problems facing society. In a technological age, solutions start with materials; with effective data infrastructure, we can discover the ones we need.

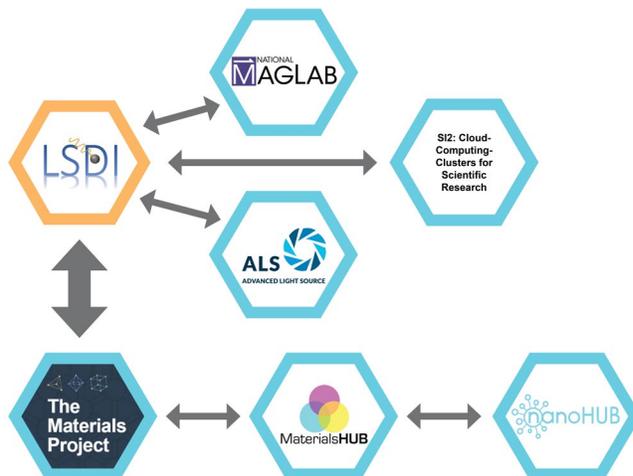


Figure 11. Part of the emerging materials research data-resource network. Image courtesy of Daryl Hess.

## Breakthrough Water Purification Technologies

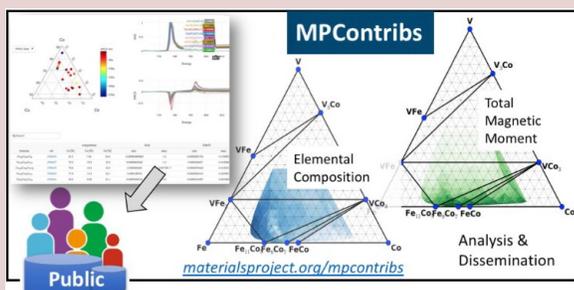
Lack of clean water and thus the consequent spreading of water-borne disease affect millions of people every year. **Benjamin Hsiao** and his colleagues at **Stony Brook University** developed new nanofibrous polymeric membranes using electrospinning. These membranes offer high water permeability, high capacity for trapping bacteria and contaminants at the nanometer range, and the ability to be manufactured economically and sustainably. These water filtration polymeric materials operate by gravity and thus do not require the expensive infrastructure, power consumption, and transmission systems of the ultrafiltration-membrane technology that is standard in all developed areas. As a result, noted paleoanthropologist and conservationist, Richard Leakey, invited Professor Benjamin Hsiao to his research institute in Kenya to explore the possible use of his materials and water-filtration apparatus in remote areas of Africa. Benjamin Hsiao's research has led to commercially available products such as nanofilter water bottles.



**Figure 12.** Benjamin Hsiao (right) visiting Richard Leakey at his paleoanthropological research institute in Kenya. Image courtesy of Professor Benjamin Hsiao.

This work was supported by the NSF EAGER grant, [DMR-1019370](#), titled “Breakthrough Concepts of Nanofibrous Membranes with Directed Water Channels for Water Purification,” and the NSF grant, [DMR-1409507](#), titled “SusChEM: Structure and Property Study of Nascent Cellulose Nanocrystals and Their Use in Water Purification.” These grants were funded by the Polymers Program (cognizant NSF Program Director, Andrew Lovinger).

## Spectroscopy Data on Demand



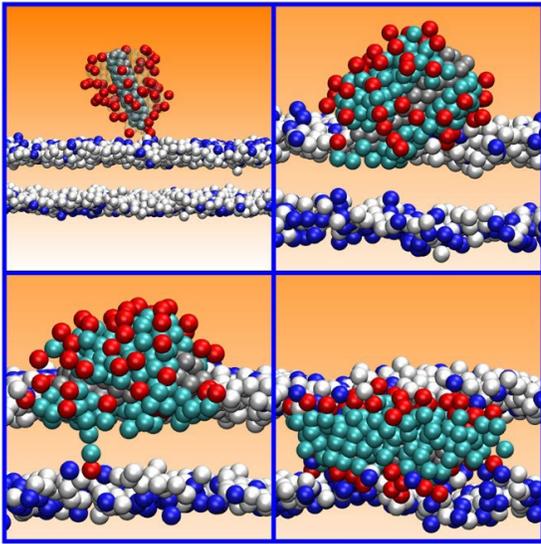
**Figure 13.** Cleaning process parameters and spectra are fed into LSDI's MPContribs environment for analysis and dissemination. MPContribs pulls calculated phase diagrams and XAS spectra from the Materials Project for interactive comparisons. Image courtesy of Kristin Persson.

The ability to access and share XAS and NMR data can lead to insights into electronic structure, bonding, and local atomic environments, and can be used to develop models to predict material structure. **Kristin Persson**, and her colleagues at the **University of California Berkley**, have developed a dissemination vehicle that can bring spectroscopy data to your desktop along with computational comparison of theory and experiment through the Local Spectroscopy Data Infrastructure (LSDI). The LSDI-developed tool, MPContribs, facilitates comparison of computed XAS spectra from the Materials Project with experimental XAS data from a major facility, such as the Advanced Light Source. Currently, the Materials Project contains computed XANES spectra for about half of the total compounds available in the database, where these spectra can be browsed and downloaded free of charge. A new XAS app allows the user to upload and

compare their own spectra with existing ones within the same chemical system to help better identify the local environment within the sample.

This work was support by the NSF award [OAC-1640899](#), titled “CIF21 DIBBS: EI: The Local Spectroscopy Data Infrastructure (LSDI).” The Office of Advanced Cyberinfrastructure, the Division of Materials Research, and the Chemistry Division contributed funds to this award (cognizant NSF Program Director, Amy Walton).

# Metaphilic Architectures for Better Antimicrobials



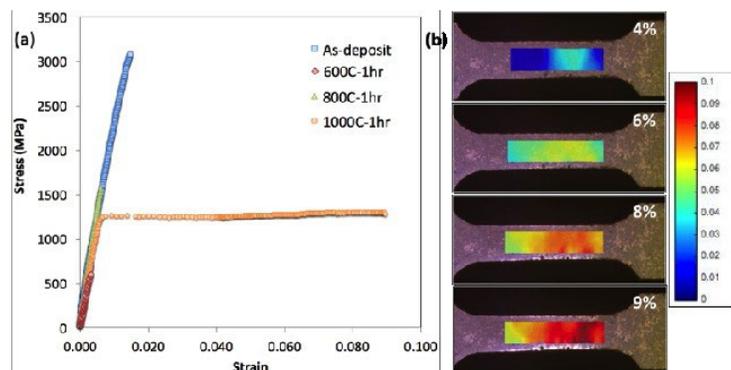
**Figure 14.** Landing and insertion process of metaphilic peptides near a membrane. Simulation images show insertion and ‘tunneling’ of side chains that lead to a fully inserted state. Image courtesy of Gerard Wong and Andrea Kasko.

The current approach to creating new antimicrobials involves using a potent broad-spectrum drug, which kills both beneficial and pathogenic species in the system. **Gerard Wong, Andrea Kasko**, and their colleagues from the **University of California Los Angeles**, enhanced the membrane-permeating activity of antimicrobial peptides and cell-penetrating peptides using a metaphilic architecture with quasi-liquid surfaces and adaptable shapes. Synchrotron X-ray scattering, cell-based studies, computer simulations, and a quantitative mean field theory were combined to show how the shape-changing properties of these peptides and the resultant adaptive presentation of chemistry played a key enabling role in their interactions with membranes. These antimicrobials from host-associated microbial communities would have the potential to regulate complex microbial colonies by inhibiting pathogenic bacteria without harming host cells or other beneficial bacteria.

This work was supported by the NSF grant, [DMR-1411329](#), titled “Toolbox for Hybrid Variable-Bandwidth Bacterio-Mimetic Antimicrobials,” and was funded by the Biomaterials Program (cognizant NSF Program Directors, Alex Simonian and Mohan Srinivasarao).

# Developing Metallic Materials for Extreme Environments

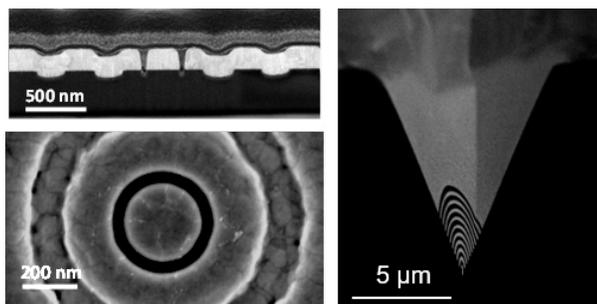
Micro-devices and microelectromechanical systems (MEMS), with sensing and guidance in harsh environments, are of interest in areas such as aviation, automotive, power generation, sub-sea drilling, and chemical processing industries, because they would provide enhanced feedback and control. **Kevin J. Hemker**, and his colleagues at **John Hopkins University (JHU)** and **General Electric Global Research (GEGR)**, developed advanced metallic materials for high temperature MEMS sensors and micro-switches. These fabricated nanotwinned nickel-molybdenum-tungsten films, with extremely high tensile strength and thermal mechanical stability, contain the presence of dense nano-twins and stacking faults. This study suggests that sputtering and subsequent heat treatment may offer an attractive option for depositing metallic MEMS materials with tailorable mechanical properties. A broader spectrum of MEMS materials would potentially offer a wider range of functionality and fuel a greatly expanded assortment of MEMS applications.



**Figure 15.** Stress-strain curve of the films annealed at different temperatures (left). Strain map of the ductile sample taken at several strain steps (right). Image courtesy of Kevin J. Hemker.

This work was supported by the NSF grant, [DMR-1410301](#), titled "GOALI: Development of Metallic MEMS Materials for Extreme Environments." This grant was funded by the Metals and Metallic Nanostructures Program (cognizant NSF Program Director, Gary Shiflet).

## Giving a “Twist” to Light-Matter Interactions



**Figure 16.** Scanning electron microscope (SEM) images of grating-flanked coaxial nano-aperture (left). SEM images of a chiral tip, which is made with focused ion beam milling (right). (Zhao Y. et al, Nature Nanotechnology, v. 12, p.1055, 2017).

The color of objects, the efficiency of solar cells, and the physics of fiber-optical communications are all interconnected by the way light interacts with materials. Light is composed of oscillating electric and magnetic fields, but at visible frequencies, most materials only interact with the electric component. Separating enantiomers, or optical isomers, is of paramount importance for the pharmaceutical and agricultural industries, but remains economically costly and time consuming with existing chemical methods. **Jennifer Dionne**, and her colleagues at **Stanford University**, developed an optical platform to separate chiral nanostructures. Their technique relies on coaxial plasmonic optical tweezers placed near a chiral mixture. When

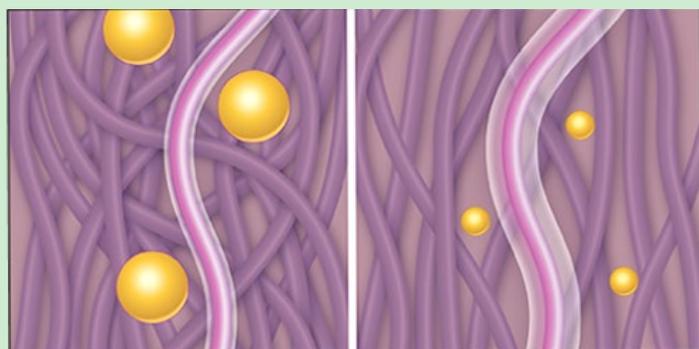
illuminated with circularly polarized light, the coaxes exert optical forces that attract one enantiomer, but repel the other. The enantioselective forces were quantified using an atomic force microscopy, laying a foundation for increasing the efficacy of pharmaceutical drugs, as well as reducing the toxicity and environmental impact of herbicides and pesticides.

This work was supported by the NSF CAREER award [DMR-1151231](#), titled “CAREER: Symmetry Breaking in Metamaterials: Giving a ‘Twist’ to Light-Matter Interactions.” This grant was funded by the Electronic and Photonic Materials Program (cognizant NSF Program Directors, Miriam Deutsch and Tania Paskova).

## Untangling Polymer Chains with Small Particles

Long polymer chains have a low mobility and tend to get entangled. The addition of nanoparticles into polymeric matrices, however, is known to lead to remarkable changes in the viscosity of the resultant composites. **Erkan Senses**, from the **University of Maryland** working at the **Center for High Resolution Neutron Scattering (CHRNS)** at the National Institute of Standards and Technology (NIST), along with his colleagues from Clemson University and Argonne National Laboratory, discovered that mixtures containing large particles have a higher viscosity, but smaller particles unexpectedly act to decrease the drag. The small nanoparticles dilate the polymer chains, pushing them apart, and increase their effective reptation diameter. The research team used the CHRNS Neutron Spin Echo spectrometer and related rheological techniques to compare the dynamics of a pure polymer relative to two polymer mixtures with three nanometer and 20 nanometer gold nanoparticles which are smaller and larger, respectively, than the voids between the polymer chains. This investigation constitutes the first observation of nanoparticle size-driven disentanglement of polymer chains, and the results could ultimately provide a path forward for controlling polymer viscosity in industrial processes such as extrusion.

This work was supported by the NSF grant [DMR-1508249](#), titled “The NIST/NSF Center for High Resolution Neutron Scattering.” This grant was funded by the National Facilities Program (cognizant NSF Program Directors, Leonard Spinu, Guebre X. Tessema, and Charles Ying).



**Figure 17.** Schematic of effective viscosity change with particle size in polymer-nanoparticle mixtures. Image courtesy of APS/Carin Cain.

# DMR Welcomes New Staff



**Dr. Eva Campo**

Dr. Eva Campo was the Opto-Nanomechanics Lecturer at Bangor University, UK prior to joining NSF. She joined DMR as Program Director in March 2017 and is responsible for managing the Partnership for Research and Education in Materials and oversees the Data efforts in the division.



**Dr. Germano Iannacchione**

Dr. Germano Iannacchione is a Professor of Physics at Worcester Polytechnic Institute. He joined DMR as Program Director in August 2017 and is responsible for co-managing the Condensed Matter Physics program.



**Dr. Gary Shiflet**

Dr. Gary Shiflet is a William G Reynolds Professor in the Department of Materials Science and Engineering at the University of Virginia. He joined DMR as Program Director in July 2017 and is responsible for managing the Metals and Metallic Nanostructures program.



**Dr. Mohan Srinivasarao**

Dr. Mohan Srinivasarao is a Professor in the School of Materials Science and Engineering at Georgia Institute of Technology. He joined DMR as Program Director in July 2017 and is responsible for co-managing the Biomaterials program and the Materials Research Science and Engineering Centers program.

## Subscribe to DMR's Mailing List

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