WINTER 2017

DMR DIVISION OF MATERIALS RESEARCH

DIRECTORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES

IN THIS ISSUE

Did You Know?

We Have a New Website

The DMR website has a new appearance.

You Can Be a Reviewer

If you would like to review DMR proposals, please complete a three-minute survey.

Program Directors Provide Feedback

Individualized comments with helpful feedback for declined proposals can be found in FastLane, between "Proposal Status" and "Reviews." Please discuss these comments with Program Directors prior to submitting a revised proposal; note that resubmitted proposals can be returned without review if they are not substantially revised.

Late Proposal Submissions Will Not Be Accepted

NSF now strictly enforces proposal submission times. A proposal must be submitted by 5:00 PM submitter's local time of the deadline date, or the proposal will not be accepted. This is now part of an AUTOMATED COMPLIANCE CHECKING procedure.

Collaborator's Information Changed

NSF PIs need to upload a single-copy document entitled "Collaborators and Other Affiliations," which is no longer required in the Biographical Sketch. Check out the Proposal and Award Policies and Procedures Guide for more information.

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.

Editor: Kelsey Smith

Letter from the Division Director

Linda Sapochak
Division Director
Division of Materials Research
National Science Foundation

Greetings,

As we commence the new year, I would like to extend my deepest gratitude for the materials research community's contributions in helping the Division of Materials Research (DMR) and the National Science Foundation (NSF) meet our mission to "promote the progress of science." Without this crucial partnership with you, we would not be able to complete our work in responsibly investing public funds to ensure the health of the U.S. research enterprise.

As a single division, DMR represents a broad and diverse research portfolio in the NSF, entertaining proposals in materials research from all physical sciences and engineering disciplines, and through multiple modes of funding mechanisms. This includes unsolicited topical materials proposals from individual investigators, team proposals through the Designing Materials to Revolutionize and Engineer our Future (DMREF), and centers programs, which include the Materials Research Science and Engineering Centers (MRSEC) and the Science and Technology Centers (STC). DMR also supports national facilities and instrumentation development at the National High

"This is an important job which is not possible without a strong partnership with you from the research communities."

Magnetic Field Laboratory (MagLab) and at the Cornell High Energy Synchrotron Science (CHESS) facility, as well as through a partnership with NIST, which supports the Center for High Resolution Neutron Scattering (CHRNS). These facilities are available at no cost to the research communities and typically serve numerous disciplines outside materials research. This exemplifies the interdisciplinary spirit that DMR was created to foster. DMR also strives to diversify and strengthen the STEM workforce through broader impact activities in all our awards, through the Partnerships in Research and Education in Materials (PREM) program and other targeted activities, and through support of summer schools, workshops, and conferences.

DMR takes very seriously our mission in serving the U.S. public to advance materials research frontiers and develop the workforce for our nation. **This is an important job which is not possible without a strong partnership with you from the research communities.**

Bearing this in mind, DMR has initiated this newsletter with the intention of better informing the materials research communities and further strengthening our partnerships as we face new challenges to our mission, both now and in the future.

This first newsletter informs you of changes at NSF affecting proposal submission and reporting, staffing and career opportunities, as well as specific changes in DMR programs and/or practices. The newsletter begins with the "Did You Know?" column to provide you with quick updates, advice, answers to commonly asked questions, and/or notices that we feel are timely and helpful to the community.

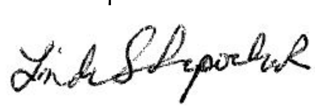
Within these pages, additional partnership building activities are featured, in which we inform you of our special activities at professional society meetings, so please take note of the events planned at the American Physical Society (APS) and the Materials Research Society (MRS) spring meetings in this issue. I strongly encourage all of you attending these meetings to participate in the NAS Decadal Review Town Hall, conducted by the National Academies to solicit input from the materials research communities. This study, Frontiers of Materials Research: A Decadal Survey, is supported by DMR and the Department of Energy's Office of Basic Energy Sciences to help us understand the changing landscape and future needs of materials research in the context of the U.S. and international efforts in important emerging research areas.

Each newsletter will feature DMR-funded research, education and facility highlights, and full articles discussing important initiatives that DMR supports. In this issue, we are featuring the National Strategic Computing Initiative, Quantum Leap, Big Data and Materials Sustainability.

The path by NSF and research communities to "promote the progress of science" has always been afforded challenges and opportunities. Let us move forward together to strengthen our partnership and seize the opportunities. I look forward to our continued partnership and wait to be amazed at what our unified efforts will produce.

Best Regards,

Linda S. Sapochak



Career Opportunities in CMP

with the NSF, DOE, AFOSR, and ONR

Tomasz Durakiewicz and Paul Sokol

Monday | March 13, 2017 | 7:30 PM - 9:20 PM

Session D22 | New Orleans Theater A

Speed Coaching

with the NSF DMR Program Directors

Velma Lawson and Elaine Washington

Tuesday and Wednesday | March 14 - 15, 2017 | Booth #141

Tuesday and Wednesday Morning Sign Up | 9:30 AM - 11:30 AM

Tuesday and Wednesday Speed Coaching | 1:30 PM - 3:30 PM

NAS Decadal Review Town Hall

The Future of Materials Research with the NSF and DOE

Thursday | March 16, 2017 | 3:30 PM

Session V7 | Room 266

Platforms Gain Momentum in the New Year

DMR has introduced a new mid-scale instrumentation program called Materials Innovation Platforms, or MIP. MIPs are national user facilities that provide free access to state-of-the-art instrumentation, tools, and expertise to advance a focused area of materials research. There are currently two Platforms: one at Pennsylvania State University (2DCC-MIP) and another led by Cornell University (PARADIM-MIP). These two Platforms focus on advancing the discovery of new two-dimensional (2D) electronic materials in thin film and bulk crystal form, with 2DCC focusing on chalcogenide materials and PARADIM-MIP focusing on heterostructures that include oxides, chalcogenides, graphene and other materials that enable novel electronic and magnetic functionalities. Access to the Platforms are via a three page scientific proposal reviewed by external experts.

These two initial Platforms focus on 2D materials for electronic applications and will serve as a nexus of expertise where users will gain access to not only mid-scale level tools, but expertise in synthesis, characterization, and theory to help design and conduct experiments. Platforms will also lead in making the data generated widely available to further accelerate the development and deployment of new 2D materials systems. What can you do at a MIP?

- Grow new 2D and related films by molecular beam epitaxy and chemical vapor depositions
- Fabricate bulk crystals for exfoliation or experiments via a variety of techniques
- Obtain pre-made 2D samples
- Obtain specialty/custom samples
- Work with a theorist to design your next material or model your results
- Send your students to free synthesis, modeling, and characterization hands-on Summer Schools
- Attend monthly virtual training from the 2DCC MIP
- Gain access to characterization techniques and data
- Gain access to models and simulation data

Take advantage of these new facilities and become part of the "community of practitioners" to advance the field of 2D and related materials for electronics!

2D Crystal Consortium
NSF Materials Innovation Platform

PARADIM
PLATFORM FOR THE ACCELERATED REALIZATION, ANALYSIS & DISCOVERY OF INTERFACE MATERIALS

DMREF Goes Biennial

This past June, the federal agencies celebrated the fifth anniversary of the Materials Genome Initiative (MGI) at the White House. In response to this initiative, the National Science Foundation (NSF) established the interdisciplinary program Designing Materials to Revolutionize and Engineer Our Future (DMREF) that encourages small academic teams to discover, design, and make materials with specific and desired functions or properties from first principles. Since its inception in 2012, the program has awarded 258 grants to teams at 80 academic institutions in 30 states. Since 2014, DMREF has been offered as a yearly solicitation; however, after the 2017 competition, the DMREF program will be offered every other year, with the next solicitation being offered in 2019.

Some Topical Materials Programs Go "Windowless"

Currently, the Division of Materials Research (DMR) has eight **topical materials programs**, including Biomaterials (BMAT), Ceramics (CER), Condensed Matter Physics (CMP), Condensed Matter and Materials Theory (CMMT), Electronic and Photonic Materials (EPM), Metals and Metallic Nanostructures (MMN), Polymers (POL), and Solid-State and Materials Chemistry (SSMC). These programs have typically accepted unsolicited proposals during an open window starting on September 1 and ending October 31. Two changes going foward are in place:

1. CER and CMMT programs will be accepting programs **anytime** following the guidelines in the corresponding solicitations found at these links, CER and CMMT, respectively.
2. All other topical materials programs will accept unsolicited proposals **once a year** between October 1 through October 31.

National Strategic Computing Initiative

Tomasz Durakiewicz

On July 29, 2015, a Presidential Executive Order created a National Strategic Computing Initiative (NSCI). The overarching goal of NSCI is to maximize the benefits of high-performance computing (HPC) research, development, and deployment. The initiative framework is based on the cooperation of three Lead Agencies: the Department of Energy (DOE), the Department of Defense (DoD), and the National Science Foundation (NSF). The Lead Agencies are supported by two Foundational Research and Development Agencies: the Intelligence Advanced Research Projects Activity (IARPA) and the National Institute of Standards and Technology (NIST). There are also five deployment agencies for the NSCI: The National Aeronautics and Space Administration (NASA), the Federal Bureau of Investigation (FBI), the National Institutes of Health (NIH), the Department of Homeland Security (DHS), and the National Oceanic and Atmospheric Administration (NOAA). Within this framework, of interagency cooperation, NSF is tasked with leading the advances in scientific discovery, promoting the broader HPC ecosystem for scientific discovery, and developing the future workforce for HPC. The importance of this fundamental research is reflected in the Executive Order through NSF's role as lead agency.

NSCI's Key Objectives

1. Accelerating delivery of a capable exascale computing system that delivers approximately 100 times the performance of current systems,
2. Increasing coherence between the technology base used for modeling and simulation and that used for data analytic computing,
3. Establishing, over the next 15 years, a viable path forward in the "post-Moore's Law era,"
4. Increasing the capacity and capability of an enduring national HPC ecosystem, and
5. Developing an enduring United States Government, industrial, and academic collaboration to ensure that the benefits of the research and development advances are shared.

Miniaturization, increasing speed, and lowering power consumption are key to future electronics. In 1965, one of Intel's co-founders, Gordon Moore, predicted that the number of transistors per unit area of a chip would double every two years. This progress of integration materialized within the last half-century, and it fueled the massive growth of the semiconductor industry, enabling modern computing. However, the limits of further miniaturization are almost reached, inhibiting continued progress. One simply cannot put in more transistors and narrow the conductors further without changing the current paradigms. The fastest computer today, the Sunway TaihuLight in Wuxu, reaches peak performance of over 93 petaFLOPS (floating point operations per second). Meanwhile, the exascale computer envisioned in Objective 1 should be capable of one exaflop, or a billion billion operations per second. Using technology available today, this computer would be the size of a football field and would consume enough power to run a city. New physics, new materials, and novel approaches could help meet this need, and the work starts from basic research.

This research is deeply fundamental in nature and problems associated with the transition from fundamental research to applications are typical for early phases of discovery. States of interest can decohere rapidly, require ultra-low temperatures, or cannot be scaled up. Therefore, substantial effort will be required to move us from fundamental research to applications. Opportunities for DMR communities will involve work where novel materials are discovered and characterized, but also where pathways toward future applications are proposed by researching options to decrease scattering, increase operational temperatures, or propose methods of scaling.

NSCI strongly couples to the "The Quantum Leap: Leading the Next Quantum Revolution" Big Idea at NSF. Specifically, Objective 3 of NSCI centers around materials development for quantum science and engineering to enable quantum-based computation. Objective 4 revolves around ecosystems, and also includes training the new "quantum workforce." Objective 5 encourages the close collaboration of industries and research required for deployment of quantum technologies. In collaboration with DOE,

"Going beyond Moore's Law and exploring the Second Quantum Revolution may be the "Apollo Project" of the coming decade, and the DMR research community has an important role to play in this voyage."

and with the help of Principal Investigators (PIs) from Massachusetts Institute of Technology (MIT), Johns Hopkins University, Cornell University and Pennsylvania State University, DMR is already active in supporting this area. DMR is organizing a Summer School on Quantum Science. It is aimed at educating graduate students in broad aspects of materials science, physics, chemistry, and engineering, while enabling good understanding of the industry practice in quantum technologies. We are also working on several other ways to advance the goals of NSCI and the Quantum Leap, so stay tuned!

Fundamental research of novel materials is the sustaining element of researchers funded by DMR. While NSF will be involved in all five objectives, DMR's specific focus and area of opportunities are related primarily to Objective 3. The success of Objective 3 depends on our ability to understand, design, develop, and control novel materials so they can effectively replace existing technology.

Some NSCI-related research is already underway in areas like topological surface states, nitrogen centers, and skyrmions. Using novel physics is a common thread among often unrelated approaches investigated here. For example, the robust nature of surface sates in topological insulators is provided via protection of those states by time-reversal symmetry. Thanks to the fundamental properties of Majorana fermions, Majorana modes are expected to provide interference-free information storage. Other exciting areas involve biological materials such as proteins, which can be manipulated into forming logic states.

Going beyond Moore's Law and exploring the Second Quantum Revolution may be the "Apollo Project" of the coming decade, and the DMR research community has an important role to play in this voyage.

Cyberinfrastructure Opportunities Advance Materials Research

Daryl Hess

The goal of the Materials Genome Initiative (MGI), announced by the White House in June 2011, is to go from materials discovery to deployment in half the time and at a fraction of the cost. The National Science Foundation (NSF) workshop, **"The Materials Genome Initiative: The Interplay of Experiment, Theory and Computation,"** held at NSF headquarters in December 2013, examined the concept of the synergistic interaction of computation, experiment, and theory, known as "closing the loop," is the foundation of the **Designing Materials to Revolutionize and Engineer our Future (DMREF)** program. Much work towards the MGI goal has been done since then through DMREF projects, investments in infrastructure, and core programs. Preparations are underway for a new workshop to be held in late spring 2017, to highlight the progress that has been made and to identify new opportunities to advance materials research.

Harnessing digital data will ultimately play a key role in achieving the goals of MGI. The Condensed Matter and Materials Theory (CMMT) program of the DMR, along with the Division of Advanced Cyberinfrastructure (ACI) and the Civil, Mechanical, and Manufacturing Innovation Division (CMMI), sponsored a workshop on the "Rise of Data in Materials Research," which took place at the University of Maryland during June 29 - 30, 2015. This workshop brought together eighty theoretical, computational, and experimental researchers from academia, industry, and government laboratories, who strived to develop a coordinated effort in understanding how to exploit opportunities and implement data-centered approaches in computational materials science. The six themes discussed reflect the opportunities and challenges in data collection, curation, management, accessibility, transformation into science, and education. The workshop was intended to start a discussion about the role of data in materials research and the opportunities findable, accessible, interoperable, and re-usable data hold for materials research. To further stimulate this discussion, a Town Hall Meeting was held in Nashville, TN, at The Mineral, Metals, and Materials Society (TMS) meeting on February 17, 2016. The meeting featured contributions from investigators across the United States, and Citrone, a materials informatics company. The Rise of Materials Research website summarizes these activities and provides resources on data for the materials research community. The website also seeks input from the community via a discussion forum. The input collected from the community will be organized in a publicly available position paper, and will ultimately become a report published as a journal article. **Be involved! Visit the Rise of Data in Materials Research website and post your comments!**

Six Themes

- The creation and use of materials cyberinfrastructures.
- Support for junior and senior researchers engaged in infrastructure creation.
- Best practices for data handling and management.
- Extraction of knowledge from data as opposed to pure data mining.
- Education of materials researchers in the age of big data.
- Development of grassroots standards and support from funding agencies.

The modern field of materials research relies increasingly on findable, accessible, and usable advanced instrumentation, computational tools, high performance computing hardware, data volumes and resources, and much more. No less important is a workforce and a research community able to use these tools effectively in advancing the frontiers of science and in capitalizing on the materials research opportunities to create new economic opportunities for our nation. Building an environment to do science that can seamlessly integrate "the loop" - computation, experimental data, and human ingenuity and creativity - depends on elements of advanced cyberinfrastructure like these, and their integration into the shared cyberinfrastructure of the materials research community. The cyberinfrastructure of the materials research community, like many, is hardly complete.

You can have an impact! ACI posted the **Dear Colleague Letter NSF 17-031: Request for Information on Future Needs for Advanced Cyberinfrastructure to Support Science and Engineering Research (NSF CI 2030)**, on January 5, 2017. Please take this opportunity to contribute to this **Request for Information (RFI)** and tell us about science challenges and cyberinfrastructure needed to engage them over the next decade and beyond. DMR, like other divisions across the Foundation, work together with ACI. Contributions to this RFI will be used during the coming year to inform the Foundation's strategy and plans for advanced cyberinfrastructure investments. We invite bold, forward-looking ideas that will provide opportunities to advance the frontiers of science and engineering well into the future.

The above Dear Colleague Letter points to an external submission website. Please note that the deadline for submissions is April 5, 2017 5:00 PM ET. Questions about this effort and the submission process should be sent to William Miller, Division of Advanced Cyberinfrastructure. Your input is important; cyberinfrastructure empowers the community to continue to do the best science.

Materials Research and Sustainable Development

Linda Sapochak and Andrew Lovinger

The Division of Materials Research (DMR) has always had an interest in sustainability-related research and environmentally benign materials. Over the years, several mechanisms have been introduced at the National Science Foundation (NSF) to encourage research in this area. One current mechanism is the Sustainable Chemistry, Engineering, and Materials (SusChEM) funding opportunity, which is described in the Dear Colleague Letter NSF 16-093. Examples of fundamental research topics in SusChEM that are of interest at NSF include: the replacement of rare, expensive, and/or toxic chemicals/materials with earth-abundant, inexpensive, and benign chemicals/materials; recycling of chemicals/materials that cannot be replaced; development of non-petroleum based sources of important raw materials; chemicals/materials for food and/or water sustainability; elimination of waste products and enhancements in efficiencies of chemical reactions and processes; discovery of new separation science that will facilitate recycling and production of valuablechemicals/materials; and development and characterization of low-cost, sustainable, and scalably-manufactured materials with improved properties. It is very important to keep in mind that the above examples include areas of sustainability that may be more appropriate for NSF Divisions other than DMR, and that any proposals to DMR must be focused on fundamental materials research aspects. It is also important to remember that principal investigators must explicitly address in the "project description" section of their proposal how their project conceptually advances sustainability in the fundamental research topics of interest in SusChEM.

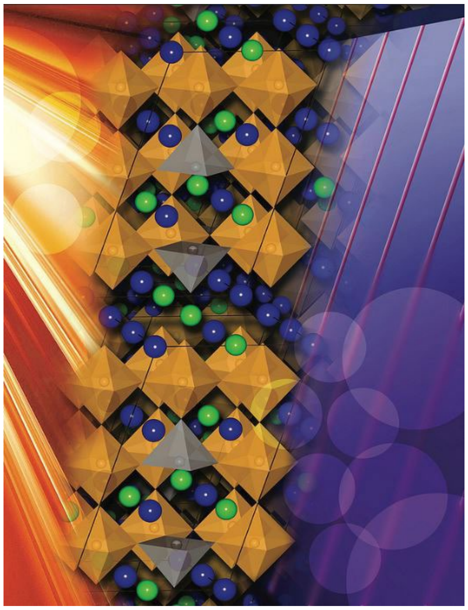


Figure 1. A perovskite crystal used in the new ceramic photovoltaic material for constructing solar panels at DOE's Argonne National Laboratory. Image credit: Felice Macera.

A second mechanism of interest at NSF is Innovations at the Nexus of Food, Energy, and Water Systems (INFEWS). The current Dear Colleague Letter NSF 17-013 introduces the NSF-wide interest in this important cross-cutting area. The need to study this interconnected water-food-energy nexus is increasingly urgent, as growing U.S. and global populations, changes in land use, and increasing geographic and seasonal variability in precipitation patterns are placing ever-increasing stress on these critical resources. NSF, through INFEWS, is uniquely poised to focus not only on the fundamental science and engineering questions at this nexus, but to train the next generation of researchers in this interdisciplinary area. Under INFEWS, foundational knowledge that leads to technological breakthroughs is of interest in the following broad areas: ensuring a sustainable water supply for agriculture; "closing the loop" for nutrient life cycles; crop protection; innovations to prevent the waste of food and energy; sensors for food security and safety; and maximizing biomass conversion to fuels, chemicals, food, and materials. Again, any proposals to DMR must be focused on fundamental materials research aspects.

Figure 2. The new, efficient oxygen catalyst in Dan Nocera's laboratory at MIT, potentially boosting solar development as a 24-hour source. Image credit: MIT/NSF.

DMR has also supported various activities promoting sustainable materials at national meetings. For example, the Materials Research Society (MRS) meetings have featured sustainability-oriented technical programming for many years, including NSF/DMR-funded symposia, forums, and tutorials. MRS has supported other related activities, including outreach and publications. The 2016 MRS Spring Meeting and Exhibit in Phoenix was the second MRS meeting to offer an entire suite of "Focus on Sustainability (FoS)" activities, including a symposium (EE15: Materials for Sustainable Development–Integrated Approaches), tutorial, professional development seminar, outreach resources and activities, and student poster competition. The meeting also debuted what has become an ongoing feature at MRS meetings, the FoS informational booth in the Hub, which offers a complete guide to MRS sustainability activities and resources and serves as a point of engagement for meeting attendees to interact with relevant MRS committee members, other volunteers, and staff. The FoS booth will continue to be the focal point for sustainability information at the upcoming 2017 MRS Spring Meeting and Exhibit in Phoenix (April 17–21, 2017). Meeting attendees are encouraged to stop by and to visit the FoS website prior to the meeting for the latest listing of sustainability-focused programming being offered.

Figure 3. Focus on Sustainabililty handout.

FoS programming at the 2017 MRS Fall Meeting and Exhibit in Boston (November 26–December 1, 2017) will include Symposium ES10: Materials Efficiency to Enable a Circular Materials Economy, which will provide a platform for materials scientists and related interdisciplinary experts to present research on sustainable materials, processing, manufacturing, and end-of-life solutions.

Finally, the MRS has taken an important step in bringing attention to its growing efforts in sustainability by creating the Focus on Sustainability (FoS) Subcommittee of the Public Outreach Committee. Dr. Ashley White, former American Association for the Advancement of Science (AAAS) Fellow in DMR and now Director of Communications at the Advanced Light Source at the Lawrence Berkeley National Laboratory, chairs this subcommittee. In recognition of the complexity of tackling sustainable development issues and the importance of materials to enabling solutions, the subcommittee seeds activities and events at MRS meetings and coordinates with MRS publications that put the materials-sustainability nexus in the spotlight.

New Methods Bridge Engineering and Humanities

Linda Sapochak

Faculty working with the Materials Research Society (MRS) and University of Florida have created a new course entitled the Impact of Materials on Society (IMOS). Using materials examples from sites as diverse as ancient Rome to Mars, this course bridges engineering and the humanities, and strives to both increase the technical literacy of the non-engineer and the social literacy of the engineer. Although the class was originally developed for traditional four-year institutions with Materials Science and Engineering Departments, significant interest has grown in finding ways to integrate this unique curriculum into two-year and K-12 institutions, which serve very diverse student populations. In July of 2016, the NSF funded an IMOS workshop at the American Association of Physics Teachers (AAPT) National Summer Meeting to work with AAPT members to determine the best approach to disseminate materials developed for this course into community colleges and K-12 schools. This included information on the course learning goals and outcomes, curriculum materials, videotaped lectures, flipped classroom movies, tests, the open source textbook etc., as well as guidance on nucleating the teaching teams and attracting students for institutions seeking to adopt the course. Working with representatives from high schools, two-year, and four-year institutions, the workshop successfully developed new ways of implementing this course. Those in attendance are currently using elements of the IMOS curriculum to supplement existing courses by augmenting the hands-on discovery of materials knowledge and providing more dynamic introductions to courses on energy, chemistry, physics, and geology. Those attending the workshop indicated that the IMOS curriculum also creates more interaction between students of different backgrounds and expands the horizons of the instructors and students. They also noted, however, that significant barriers remain in high schools and two-year institutions to implementation of the course materials, such as faculty overload with existing mandatory courses, matriculating the coursework for university credit, and administrative buy-in. To address these outstanding challenges, an outcome of the workshop was to nucleate a new task force of the MRS IMOS subcommittee that focuses on delivering educational content to high schools and two-year institutions. The mandate for this task force is to develop new and innovative ways of supporting teachers in integrating materials developments into curricular and extracurricular activities. The task force is made up of representatives from K-12 and community college institutions, and they are excited to be working to leverage the educational and outreach arms of the MRS in order to connect MRS local chapters and materials scientists to reach a more diverse student group earlier in their studies. Thanks to the vital seed funding by the NSF, this conversation about implementing socially-engaged materials curriculum into two-year institutions has grown into a larger committee looking at enriching K-12 and community colleges not only domestically, but also internationally.

> Using materials examples from sites as diverse as ancient Rome to Mars, this course bridges engineering and the humanities.

This work was supported by the NSF grant DMR-1449542, titled "Impact of Materials on Society (IMOS) Workshop," and the NSF grant DMR-1643044, titled "Dissemination of the Impact of Materials on Society (IMOS) Course through a Workshop at the AAPT" and funded by the XC program (formerly referred to as the Office of Special Programs) (cognizant Program Director, Lynnette Madsen). Kevin S. Jones, the Principal Investigator, Fredrick N. Rhines (University of Florida), and the co-Principal Investigator, Sophia Krzys-Acord (University of Florida), worked closely with Bart Sheinberg (Houston Community College) and Pamela Hupp, (MRS) on these projects.

Novel Approach to Fighting Decoherence in Molecular Spin Qubits

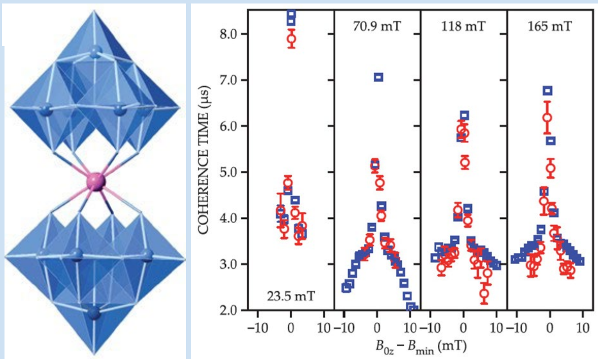


Figure 1. Left: HoW10 molecule. Right: Increased coherence observed at four different clock transitions, with red and blue data points corresponding to the measurements at 9.1 GHz and 9.2GHz, respectively. Magnetic fields of transitions are shown in each panel, with deviations from each respective value shown in horizontal axis.

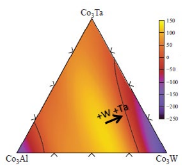
Future quantum computers will require stable and decoherence-free qubits. Magnetic molecules offer a useful and widely researched platform for such qubits, but the lifetimes of useful quantum states are limited by magnetic interactions. Separation in space minimizes the interactions and reduces decoherence, but leads to low density of qubits, which in turn makes it more difficult to perform quantum operations based on the interaction between qubits. Results of recent work by Stephen Hill and collaborators show how to minimize decoherence without dilution of spins. In this novel approach, the molecules are tailored to protect their spin dynamics from decoherence related to spin-spin interactions, allowing high density of qubits with long coherence times to exist in close proximity while avoiding the spin noise. The approach is based on optimization of operating points, or atomic clock transitions, by using crystal field ground states with large tunneling gaps that are resistant to dipolar decoherence. Such "sweet spots" allow the information-carrying spin states to be insensitive to magnetic noise. The method was tested on a holmium molecular nanomagnet system using electron paramagnetic resonance, where record-long coherence times of several microseconds were obtained at high concentrations.

This work was supported by the NSF grant DMR-1309463, titled "High Frequency EPR Studies of Strong Spin-Orbit Effects in Molecular Magnetism" and funded by the CMP Program (cognizant Program Director, Tomasz Durakiewicz). The measurements were performed at the National High Magnetic Field Laboratory (NHMFL). NHMFL is supported by the NSF grant DMR-1157490 (cognizant Program Director, Leonard Spinu). Stephen Hill (Florida State University) was the Principal Investigator and results of this research were published in the following reference: "Enhancing coherence in molecular spin qubits via atomic clock transitions." Muhandis Shiddiq, Dorsa Komijani, Yan Duan, Alejandro Gaita-Ariño, Eugenio Coronado and Stephen Hill. *Nature* 531, 348–351 (2016).

High Temperature Materials Ready for Take-off

When it comes to aircraft engines, rocket motors, and nuclear power plants, the "heat" is constantly on to make the parts inside stronger, more reliable, and more durable. In fact, when an airplane takes off, the materials in the hottest part of the engine reach about 90 percent of their melting temperature, so there's always a desire to find a material that can operate at a higher temperature. Materials scientist, Tresa Pollock, and a team at the University of California, Santa Barbara, are partnering with General Electric and others to develop new multilayered materials designed for high performance in extreme environments. Pollock's team is pioneering the use of new modeling tools to speed up the development process and using advanced

Computation



Experiment

Materials

computer algorithms and Big Data analysis to hone their designs before testing them. They've also designed and built a custom microscope that combines electron, ion, and laser beams to analyze the new materials for defects at the nanometer scale in 3-D. This addition of the laser speeds up the process of gathering the information; what used to take six to nine months now takes a couple of days.

This work was supported by the NSF grant DMR-1233704/DMR-1534264, titled "DMREF/GOALI - Discovery, Development, and Deployment of High Temperature Coating-Substrate Systems" and funded by the DMREF Program (cognizant Program Directors, John Schlueter and Susan Dexheimer). Tresa Pollock (University of California Santa Barbara) was the Principal Investigator and Matthew Begley (University of California Santa Barbara), Linda Petzold (University of California, Santa Barbara), Anton Van der Ven (University of California, Santa Barbara), and Frederic Gibou (University of California Santa Barbara) were the Co-Principal Investigators. General Electric was the industrial partner.

Video 1. New Multilayered Materials Ready for Take-off

World's Strongest Magnet for Nuclear Magnetic Resonance

Figure 1. The Series-Connected Hybrid (SCH) magnet during installation.

A new ultra-high-field magnet providing 36 T was completed at the National High Magnetic Field Laboratory (NHMFL). This achievement is the culmination of ten years of work by a team of more than 40 people developing this new system. The new hybrid magnet uses a novel approach where the resistive and superconducting coils are connected electrically in series. This Series-Connected Hybrid (SCH) configuration ensures a very high temporal stability of the magnetic field that enables new frontieres in high field Nuclear Magnetic Resonance (NMR). This SCH magnet is able to reach 36 T while consuming less than half the power that would be required by an all-resistive magnet. This will enable experiments that run at intense magnetic fields for many hours to be performed that would be prohibitively expensive otherwise. Another unique feature of this magnet is that it is designed to achieve high field homogeneity. Once that specification is achieved, the magnet will be used to extend Nuclear Magnetic Resonance from 23.5 T to 36 T. Working at higher fields extends the reach of NMR further into the periodic table. Much of biological chemistry involves oxygen, which has been out of range of existing NMR magnets. In addition, elements including zinc, copper, aluminum, nickel, and gadolinium – all of interest for battery and other materials research – will now be observable using the SCH magnet. The SCH magnet reached its specified peak field of 36 teslas, on November 8, 2016. Over the next period, NHMFL will be installing NMR instrumentation in preparation for the unique scientific program envisioned for this magnet.

The design and construction of the SCH was supported by the NSF through the Instrumentation for Materials Research – Major Instrumentation Projects (IMR-MIP) program, NSF grant DMR-0412169, titled "IMR-MIP Series Connected Hybrid," and NSF grant DMR-0603042 titled, "IMR-MIP Series Connected Hybrid Construction Phase" (cognizant Program Director Guebre X. Tessema). NHMFL is supported by the NSF grant DMR-1157490 (cognizant Program Director, Leonard Spinu).

Job Opportunities in DMR

DMR is dynamic. Every year, new scientists join DMR as Program Directors rotate out or leave NSF for various reasons. If you are interested in joining DMR, please send your resume to DMR-recruit@nsf.gov. We welcome applicants in all fields of materials research, as unexpected needs often arise. The website provides some useful information about working here at NSF. If you have any questions, please feel free to contact some of our current and former DMR Program Directors.

NSF Director's Award for Distinguished Service

DMR's Dr. Andrew Lovinger was awarded the NSF Director's Award for Distinguished Service for 2016. He received this award in recognition of his exceptional service to Polymer Science, the DMR, the Directorate for Mathematical and Physical Sciences (MPS), and the NSF, as well as his long-term dedication as a scientist, program director, mentor, and advisor to the mission of the Foundation.

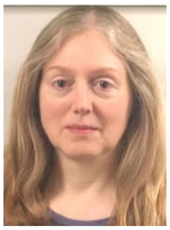
The American Ceramics Society Board of Directors

DMR's Dr. Lynnette Madsen was inducted as a member of the Board of Directors for the American Ceramics Society. Her term started October 27, 2016, and will run for three years. The American Ceramic Society's Board of Directors is responsible for setting policy, approving a budget, making appointments to leadership, and conferring awards, to name a few of its duties.

Please Welcome Our New Staff!

New Staff

Dr. Jose Alfredo Caro
Dr. Jose Alfredo Caro is a Research Scientist in the Center for Materials at Irradiation and Mechanical Extremes at Los Alamos National Laboratory. He joined DMR as Program Director in October 2015 and is responsible for managing the PREM program.



Dr. Susan Dexheimer
Dr. Susan Dexheimer is an Associate Professor in the Department of Physics at Washington State University. She joined DMR as Program Director in July 2016 and is responsible for co-managing the Designing Materials to Revolutionize and Engineer Our Future program.

Claudia Johnson
Claudia Johnson is a Contractor from InfiniSource Consulting Solutions, Inc. She joined DMR in April 2016.

Dr. Tania Paskova
Dr. Tania Paskova is a Research Professor in the Department of Electrical and Computer Engineering at North Carolina State University. She joined DMR as Program Director in September 2015 and is responsible for co-managing the Electronic and Photonic Materials program.

Allison Smith
Allison Smith is a Program Specialist. She joined DMR in July 2016.

Dr. Leonard Spinu
Dr. Leonard Spinu is a University Research Professor in the Department of Physics at the University of New Orleans. He joined DMR as Program Director in August 2015 and is responsible for co-managing the National Facilities and Instrumentation program.

Elaine Washington
Elaine Washington is a Program Specialist. She joined DMR in October 2015.

Dr. Miriam Deutsch
Dr. Miriam Deutsch is a Professor in the Department of Physics at the University of Oregon. She joined DMR as Program Director in January 2016 and is responsible for co-managing the Electronic and Photonic Materials program.

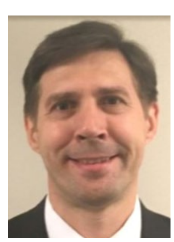
Dr. Diana Farkas
Dr. Diana Farkas is a Professor in the Department of Materials Science and Engineering at Virginia Tech. She re-joined DMR as Program Director in September 2015 and is responsible for managing the Metals and Metallic Nanostructures program.

Dr. Alexios Klironomos
Dr. Alexios Klironomos is an Associate Editor of the Physical Review B. He joined DMR as Program Director in July 2015 and is responsible for co-managing the Condensed Matter and Materials Theory program.

Dr. Birgit Schwenzer
Dr. Birgit Schwenzer is a Scientist in the Physical and Computation Science Directorate at the Pacific Northwest National Laboratory. She joined DMR as Program Director in June 2016 and is responsible for co-managing the MRSEC and Solid-State and Materials Chemistry programs.

Kelsey Smith
Kelsey Smith is a Student Program Assistant PATHWAYS Intern. She joined DMR in October 2016.

Aubrie TenEyck
Aubrie TenEyck is a Contractor from InfiniSource Consulting Solutions, Inc. She joined DMR in April 2016.



Dr. Eugene Zubarev
Dr. Eugene Zubarev is an Associate Professor in the Department of Chemistry at Rice University. He joined DMR as Program Director in July 2016 and is responsible for co-managing the Solid-State and Materials Chemistry program.

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