Introduction & History

The Center for Nanoscale Science exploits unique capabilities at Penn State and partner institutions in materials synthesis, fabrication, and assembly, physical property measurements, computation and theory to make and organize nano-materials in configurations that can attain new regimes of properties and functionality. Interdisciplinary teams attack problems in strain and layer enabled multiferroics, powered nano-scale motion, the behavior of electrons in one-dimensional materials, and the control of light in nanostructures. Center activities overall involve approximately fifty students and post-doctoral fellows, faculty from seven academic departments, and a number of external academic and industrial partners.

The Center was established in 2000 as a single Interdisciplinary Research Group, Center for Collective Phenomena in Restricted Geometries (DMR 0080019). In 2002, the Center merged with a new MRSEC, Center for Molecular Nanofabrication and Devices (DMR 0213623) comprising two IRGs: Chemically Advanced Nano-lithography (IRG1) and Nanoscale Motors (IRG2). The two MRSECs then merged. In 2004–05, the original IRG phased out its effort in fluids and polymers and split into IRG3 (Electrons in Confined Geometries) and IRG4 (Electromagnetically Coupled Nano-structures). In 2007, a new IRG on Strain Enabled Multiferroics, which grew from a seed project, was added as IRG5. In 2008, the Center was competitively renewed as a four-IRG MRSEC (DMR 0820404), in which Chemically Advanced Nanolithography phased out and Strain Enabled Multiferroics became the new IRG1.

Currently, the four IRGs investigate emergent behavior of nanoscale systems with common themes of new materials synthesis and nanofabrication, theory-led design, and length scale-dependent physical phenomena. The scientific programs of the IRGs are complemented by a highly competitive Seed program. The Seed program has played a major role in the scientific evolution of the Center, supporting junior faculty and high risk projects. Seed grants typically support 1 to 3 graduate students over ~18 months. The Seed program leverages funding from the Penn

IRG1, Atomic Scale Design of Multiferroics, focuses on new phenomena multiferroic materials in which two or more ferroic (ferroelectric, ferroelastic, magnetic) order parameters co-exist within a single material. Precise tuning is imparted by control of strain, layer stacking, gradients, and exploitation of roto symmetries. Our expertise spans from first principles and phase-field modeling predictions of new materials and phenomena, to synthesis, structural electrical, magnetic, and optical characterization, and prototype devices. Recently, the IRG has discovered thermotropic phase boundaries in lead-free classic ferroelectrics that show strongly enhanced properties in intermediate phases, new low-loss tunable dielectrics for microwave applications, and revealed atomic-scale mechanisms of ferroelectric switching.
Executive Summary

State Materials Research Institute (MRI), the Huck Institutes for the Life Sciences, and the Penn State Institutes for Energy and the Environment. In 2013, the Center refocused Seed support onto an effort in 2D magnetism which is searching a new class of new tunable magnetic semiconductors, guided by a combination of first-principles theory, chemical intuition, and cutting edge synthesis techniques.

Education & Outreach
During the past year, the MRSEC has continued to offer a range of educational outreach activities at the elementary, high school, college, and post-college levels. The majority of MRSEC faculty and graduate students have participated in at least one educational outreach program within the last year. These programs have reached approximately 3,500 K-12 students, 29 K-12 teachers, 24 undergraduates, and ~100,000 visitors to science museums over the past year. The Center’s K-12 programs increase interest in science and build confidence, with special attention towards including women at all career stages and under-represented minority high school students.

IRG2, Powered Motion at the Nanoscale, designs, fabricates, measures and models molecular and nanoscale motors to address one of the grand challenges in science and engineering, namely, to master energy transduction and information on the nano- and microscale to ultimately create new technological capabilities that rival those of living things. The IRG synthesizes and studies a range of molecular and nanoparticle-based motors that are driven by external fields, acoustic energy, and chemical reactions. Recently, we have quantified the efficiencies of the catalytic motors and increased it 1000-fold with selective bipolar reactions. We have also extracted the force/distance relation for motor-motor interactions, further developed acoustic propulsion to show activity within living cells and selective addressing based on resonance. New discoveries on enzyme motors reveals that turnover of the enzyme can generate sufficient force to cause directional movement in a gradient, with potential application in pumps. We have also developed polymer pumps that show memory effects.

IRG3, Charge and Spin Transport in Quasi-1D Nanowires, brings together complementary expertise to explore new phenomena and critically examine issues related to charge and spin transport in quasi-1D metallic, superconducting, and magnetic nanowires and nanowire junctions, phenomena that encompass low dimensional condensed matter physics, materials growth and processing, and device design and fabrication. Recently, the IRG has shown that we can induce the switching between a resistive and a non-resistive state in a cm-long quasi-1D superconducting Ga-In nanowire by the addition of a single flux quantum. The quasi-1D geometry is crucial; in 2D or 3D a single fluxon does not cause a step change in the resistance. The long length of the wire is also important, because the effect depends on a rare configuration of a pair of Ga nanodroplets in close proximity. Also, individual quantum phase slips were detected in the nanowire by means of a novel single-shot voltage measurement protocol. Recent results on the novel proximity effect in superconducting/ferromagnetic nanowires provides evidence for triplet induced superconductivity in the ferromagnet.
Executive Summary

IRG4, *Electromagnetically Coupled Nanostructures*, integrates metals, semiconductors, and dielectrics on sub-wavelength scales to access new optical and optoelectronic material properties and novel devices. Using high-pressure fluid deposition (developed in the IRG), fiber pore arrays are filled by semiconductors and metals with nanometer-scale precision over meter lengths. Semiconductors and metals have been integrated in the extreme-aspect ratio pores of microstructured optical fibers and new all-fiber optoelectronic and nanoscale imaging devices that exploit E-M coupling at dimensions down to the nanoscale and lengths up to meters are being developed. Genetically-inspired feed forward design methods are being used to create planar metallo- and all-dielectric nanostructures with user-defined E-M scattering. New passive and active (tunable) infrared and visible devices including wavelength-selective filters and mirrors, and entirely new materials with customized refractive indices including zero and negative index have also been realized.

In October 2013, the museum kit *Pocket Tech*, which explores the technology contained within personal electronic devices was distributed to 16 science museums nationwide. All demonstrations are designed to be hands-on, interactive, visual, and tactile. MRSEC members provided the initial inspiration and content ideas, feedback during the development process, ongoing technical oversight, and supplemental “fact sheets”. Several MRSEC graduate students created prototype devices which were tested by staff at the Franklin Institute and modified to become permanent designs.

The MRSEC serves as a hub K-12 outreach activities at Penn State. Center members engaged in numerous outreach activities to K-12 students, teachers, and members of the general public, including NanoDays (>600 children and adults), Kids Day for the Central Pa Festival of the Arts (11 booths, ~1000 kids), and at tailgate before a Penn State home football game with *Pocket Tech* kits (~100 fans), a Science Cafe, work with the local Discovery Space science museum, and after school programs with hands-on activities to elementary and middle school at-risk youth from the local Centre County region. MRSEC volunteers also also presented at multiple local elementary schools.Twenty three Pennsylvania K-12 educators learned about nanoscale science and technology via a one-day workshop.

Center volunteers hosted a diverse group of 25 high school aged youth at the Science Leadership Camp: Elements of Innovation, a weeklong residential experience created by MRSEC for the Science-U summer camps at Penn State, giving them a snapshot of research in microfluidic devices and graphene and networking in a “scientist mixer”, which has become a camp highlight.

The Center continues to foster active involvement of undergraduates and high school teachers through its REU/RET site, which was jointly run with the Penn State Physics Department. Representation from women and minorities in the REU and RET programs continues to be strong. Through its Diversity Committee, the Center joins forces with relevant departments, colleges, and minority-focused organizations at Penn State in fostering exchange of faculty and recruiting graduate students from minority-serving institutions. Initiatives this year include the launch of the the STEM Open House (initiated by the MR-
SEC), a partnership with the new Millennium Scholar program with MRSEC labs hosting first-year summer research experiences and the MRSEC-initiated Women in STEM Mixer. Programs continue to be actively evaluated.

The Center employs a number of postdoctoral fellows as researchers whose activities span several projects within the IRGs, and also as coordinators of education and outreach activities. The education-outreach postdocs are supported in multifaceted career-development activities.

**Knowledge Transfer & International Collaborations**

The outreach and knowledge transfer of the Center is driven primarily through research collaborations between its members with scientists and engineers in industry and national laboratories. One of the important vehicles for collaboration with industry is the MRSEC’s Industrial Affiliates Program, now in its seventh year, with corporate members who jointly support the work of students in the Center. Further research is supported by industrial consortia or in partnership with start-up companies. In addition to research collaborations, MRSEC faculty play a leading role at Penn State in organizing industrial workshops, making presentations at workshops and conferences, and participating in industrial fellowships and internships. The MRSEC also hosts a number of visiting scientists and is a strong component of the overall industrial/technology transfer infrastructure of the University. There is also strong international component to collaborative research and outreach activities of the Center.

**Management**

The management structure centers around the Executive Committee, Director, Associate Director and the IRG leaders with well-defined responsibilities as outlined in later sections. The Director reports regularly to the Executive Committee and the Vice President for Research, and consults with the directors of the Penn State Institutes (MRI, PSIEE, Huck). The Executive Committee meets about once a month, often after the Monday lunch seminars to discuss scientific progress of the various projects, review requests for substantial resource allocation, and discuss optimal strategies to maintain constant growth and renewal of our research and outreach missions. The Executive Committee is spearheading preparations for the NSF renewal.

The Penn State MRSEC is advised by an external Advisory Board, which visits bi-annually, alternating with NSF-appointed site visit teams. The Advisory Board has recently been reconstituted in preparation for the renewal, to reflect the new composition of the new proposed IRGs. Annual reviews provide a valuable external assessment of the scientific direction and administrative structure of the Center.

**Central Facilities Laboratory**

The MRSEC maintains a Central Facilities Laboratory, centrally located for easy access to all members of Center. The CFL has acquired instrumentation to serve the research needs of the four IRGs, and its facilities dovetail with the extensive facilities of the Penn State Materials Characterization Laboratory (MCL).

The Center receives supplemental funding from DMR as part of the Materials Research Facilities Network (MRFN) to support a one-day characterization workshop and a summer faculty internship program that are intended to increase the participation of faculty and students from predominantly undergraduate and minority-serving institutions in the re-
Executive Summary

These activities leverage the full suite of characterization and fabrication tools available in the CFL and MCL.

**Key Accomplishments**

**Intellectual Merit.** The Penn State MRSEC is pleased to report a number of exciting scientific accomplishments within the past year. Space limits prevent a thorough summary here: please refer to the detailed writeups.

★ In the multiferroics project of IRG1, several important discoveries were made. The IRG has discovered strongly enhanced properties in intermediate phases of thermotropic phase boundaries in lead-free classic ferroelectrics. New low-loss tunable dielectrics for microwave applications have been discovered. The IRG has also performed the first real-time, atomic-scale observations and phase-field simulations of domain switching dominated by pre-existing, but immobile, ferroelastic domains. The study provides an atomic level explanation of the hindering of ferroelectric domain motion by ferroelastic domains.

★ The IRG team has quantified the efficiencies of the catalytic motors and increased it 1000-fold with selective bipolar reactions that make more efficient use of available reagents. We have further developed acoustic propulsion to show activity within living cells. Structured polymeric bubble-powered acoustic motors have been developed that are selectively addressable through acoustic resonance. Turnover of enzyme ‘motors’ can generate sufficient force – through currently unknown, novel mechanisms – to cause directional movement in a gradient at the single-molecule level. New theoretical methodologies enable complex motors with multiple elementary motive processes to be described very efficiently within a novel matrix-based kinematrix approach.

★ There have been several new advances in the area of charge and spin transport in quasi-1D nanostructures in IRG3. The IRG has induced switching in a cm-long quasi-1D superconducting Ga-In nanowire by the addition of a single flux quantum. Individual quantum phase slips were detected by means of a novel single-shot voltage measurement protocol. The novel proximity effect in superconducting/ferromagnetic nanowires has provided evidence for triplet induced superconductivity in the ferromagnet.

★ The Center has continued to make significant advances in nanostructures grown in mesostructured optical fibers (MOFs) and planar metallodielectrics in IRG4. It now appears that HPCVD opens the possibility for deposition in many confined geometries other than optical fibers of considerable scientific and technological interest. For example, it is possible to deposit in planar geometries as long as one of the reactor dimensions is kept small enough (~10 to 100 µm) to preclude nucleation and growth of nanoparticles in the gas phase. Using a tapered Ge-infiltrated silica holey fiber array and treating each Ge fiber as a pixel to transmit infrared light, we have recently demonstrated infrared imaging spectroscopy. We have successfully designed, fabricated, and characterized optical electromagnetic bandgap metamaterial coatings with near-perfect absorption over broadband ranges with greater than an octave of bandwidth and wide fields-of-view.

**Broader Impact.** The Center continues to serve as a hub for connecting students, post-docs, and faculty at Penn State to a wide range of outreach educational and outreach activities. The Center’s outreach targets the audience of many by engaging the complementary skills of partner institutions, such as the museum shows in partnership with the
Franklin Institute. These museum shows at the Franklin and two dozen partner science museums were estimated to reach over 100,000 participants in 2013. The Center’s outreach also targets the audience of one, through hands-on research experiences, summer camps, workshops, and local events that benefit both participants and student mentors from the Center. In 2013, the fifth kit/show was distributed to 16 partner museums nation-wide. The Science Leadership Camp included a very successful evening mixer between the campers and MRSEC scientists at all levels. The Center continues to work energetically to increase the participation of women and under-represented minorities at all levels, spearheading the STEM Open House graduate recruiting event. At the K-12 levels, diversity-focused activities included the science leadership camp and guided inquiry summer laboratory experiences for high school students from disadvantaged schools through the Upward Bound program. The Center’s REU program continues to be strongly diversity-focused, leveraging partnerships with minority-serving institutions.
2. List of Center Participants

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<tr>
<th>Bioengineering</th>
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<tr>
<td>Peter Butler</td>
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<td>Chemical Engineering</td>
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<td>Kyle Bishop</td>
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<td>Ali Borhan</td>
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<td>Enrique Gomez</td>
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<td>David Allara</td>
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<td>John Asbury</td>
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<td>John Badding</td>
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### Materials Science and Engineering

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<td>Long-Qing Chen</td>
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<td>Venkatraman Gopalan</td>
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<td>Roman Engel-Herbert</td>
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<td>Suzanne Mohney</td>
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<td>Susan Trolier-Mckinstry</td>
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<td>Joan Redwing</td>
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<tr>
<td>Ron Redwing</td>
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### Physics

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<td>Moses Chan</td>
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<td>Vincent Crespi</td>
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<td>Eric Hudson</td>
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<td>Jainendra Jain</td>
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<td>Qi Li</td>
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<td>Nitin Samarth</td>
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<td>Jorge Sofo</td>
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<td>Mauricio Terrones</td>
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<tr>
<td>Jun Zhu</td>
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Jayatri Das (Education) Franklin Institute (Received Center Support in a subcontract)
Steven Snyder (Education) Franklin Institute (Received Center Support in a subcontract)
Craig Fennie (IRG 1) Cornell University (Received Center Support in a subcontract)
Darrell Schlom (IRG 1) Cornell University (Received Center Support as a co-advisor of 2 students working in IRG 1 with Long-Qing Chen)
Xiaoqing Pan (IRG 1) University of Michigan (Received Center Support in a subcontract)
Karin Rabe (IRG 1) Rutgers University (Received Center Support in a subcontract)
Ramesh Ramamoorthy (IRG 1) UC Berkeley (Received Center Support in a subcontract)
3. List of Center Collaborators

<table>
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<tr>
<th>Collaborator</th>
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<th>Field of Expertise</th>
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<tr>
<td>Timothy Bunning</td>
<td>Air Force Research Lab.</td>
<td><a href="mailto:Timothy.bunning@wpafb.af.mil">Timothy.bunning@wpafb.af.mil</a></td>
<td>Polymer</td>
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<tr>
<td>Yu-Chang Chen</td>
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<td>Electron Transport</td>
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<tr>
<td>Chi-Wen Cheng</td>
<td>National Chiao Tung University</td>
<td><a href="mailto:chiwing.ac96g@nctu.edu.tw">chiwing.ac96g@nctu.edu.tw</a></td>
<td>Ultrastable IRG</td>
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<tr>
<td>Ulbaldo M. Cordova-Figueroa</td>
<td>University of Puerto Rico-Mayaguez</td>
<td><a href="mailto:ubaldom.cordova@upr.edu">ubaldom.cordova@upr.edu</a></td>
<td>Modeling</td>
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<tr>
<td>Misaell Diaz</td>
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<td><a href="mailto:misael.diaz@upr.edu">misael.diaz@upr.edu</a></td>
<td>Modeling, Bacterial Motility</td>
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<td>Nicholas Fang</td>
<td>MIT</td>
<td><a href="mailto:nicfang@mit.edu">nicfang@mit.edu</a></td>
<td>Nanophotonics</td>
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<tr>
<td>Leonhard Grill</td>
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<td><a href="mailto:leonhard.grill@physik.fu-berlin.de">leonhard.grill@physik.fu-berlin.de</a></td>
<td>Nanocar Analysis</td>
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<td>Noel Healy</td>
<td>University of Southampton</td>
<td><a href="mailto:nvh@orc.soton.ac.uk">nvh@orc.soton.ac.uk</a></td>
<td>Nonlinear Photonics</td>
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<td>Lin He</td>
<td>Beijing Normal University</td>
<td><a href="mailto:helin@bnu.edu.cn">helin@bnu.edu.cn</a></td>
<td>Electrical Transport</td>
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<td>Martin Holt</td>
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<td><a href="mailto:mvholt@anl.gov">mvholt@anl.gov</a></td>
<td>Nanoscale xray imaging</td>
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<tr>
<td>Mauricio Hoyos</td>
<td>ESPCI (Paris Tech)</td>
<td><a href="mailto:hoyos@pmmh.espci.fr">hoyos@pmmh.espci.fr</a></td>
<td>Colloidal Particles</td>
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<td>Jiamian Hu</td>
<td>Tsinghua University</td>
<td>hjm08mails.tsinghua.edu.en</td>
<td>Phase Field Modeling</td>
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<td>Ilia Ivanov</td>
<td>Oak Ridge National Lab.</td>
<td><a href="mailto:ivanovin@ornl.gov">ivanovin@ornl.gov</a></td>
<td>Hybrid Nanostructures</td>
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<td>Stanislav</td>
<td>Academy of Sciences,</td>
<td><a href="mailto:kamba@fzu.cz">kamba@fzu.cz</a></td>
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<td>High Harmonic Generation/hollow Waveguides</td>
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4. Strategic Plan

Development of Center Vision and Mission: Nanoscale science is a rich field that is transforming materials science, not only by providing materials with enhanced properties for traditional applications but also by providing access to wholly new, transformational physical phenomena. Over the next decade, nano-materials are expected to play an increasingly important role in energy conversion, electronics, biology, environmental technology and other fields. In large measure the success of these applications depends on innovation in materials discovery and assembly, and especially on understanding of new physics that is unique to the nanoscale. Recognizing the importance of the connection between emerging science and societal benefit, the mission of the Center is to design and discover materials with fundamentally new physical properties and functions, focusing especially on phenomena that are unique to nanoscale dimensions. Success in this effort requires the participation of multi-disciplinary teams that combine expertise in materials synthesis, fabrication, theory and computation, physical property measurements and device engineering. Projects in the Center are expected to be at the forefront of their field scientifically, to be intrinsically interdisciplinary and in appropriate cases to transition to practical technology. Considering the scale of the Center, the projects should assume greater risk and ambition than a typical single-investigator effort. Renewal of the Center’s scientific focus is driven by new discoveries in the interdisciplinary research groups, and by a robust seed program that draws on talent from a large pool of materials researchers at Penn State and collaborating institutions. Periodic internal review of all programs is an important factor in maintaining the high quality and productivity of Center research. Center research is integrated with educational and industrial outreach that is designed to engage all its members and leverages the expertise and distribution networks of several partner organizations: these efforts are seen as valuable not only for the recipients (the public, students, industry) but also for the participants, as career development experience in communicating and translating research towards larger societal needs. The Center supports the career development of young scientists and those from under-represented groups through its seed program, internships, coordination with departmental admissions committees, research experiences, participation in the materials facilities network, support of a nascent science exposition for graduate-school-bound seniors, and outreach activities, as described in the Diversity Strategic Plan. This management philosophy and strategic plan for the Center has been developed jointly by the members of the IRGs, who meet weekly for seminars and informal discussions, by the past and present Center directors, and by the Executive Committee. It is expected that the future vision for the Center will continue to evolve with bottom-up input from its creative and energetic membership.

Research Goals: Transformed by the injection of new ideas and new participants, the topical emphasis of the IRGs has changed substantially since the Center’s establishment. The core research goals of the Center in hard and soft materials were re-defined by the four IRGs in the competitive renewal process of 2008. In initiating new projects and evaluating continuing ones, the Center responds to new scientific opportunities and societal needs by exploiting synergistic collaborations across fields. The following provides a picture of the Center’s current activities and research goals for the next two years:

IRG1 focuses on strain tuning and layer tuning and resulting new phenomena in complex oxides in which two or more ferroic (ferroelectric, ferroelastic, magnetic) order parameters exist within a single material. The intricate coupling between spin-charge-and-lattice degrees of freedom give rise to a rich spectrum of new phenomena and cross-coupled properties with fundamental
scientific merits on their own, as well as potential applications in highly tunable electronic and optical properties, and electrical control of magnetism. Predictive theory closely coupled to experiment plays a crucial role in these studies. Recently, this IRG has applied new focus on new classes of layered oxides that provide compelling new opportunities to exploit novel mechanisms to couple spin, charge and lattice degrees of freedom.

**IRG2** focusses its efforts onto catalytic nano/microscale motors that employ catalytically driven ion flow, hydrolysis, and acoustic energy, spanning the full range from design, to fabrication and modeling, inspired by the dynamic interplay of nanomachines that comprise living systems. This research will advance the fundamental understanding of nanomotor design to enable applications in the dynamical organization of nanomaterials and nanosystems, separations, sensing, actuation and biomedicine. Particular focus will be placed on collective interactions between motors, and the extension of motor functionality by incorporation of internal state variables. New motors types powered by acoustic fields are also being developed, including dual chemical and acoustically powered motors.

**IRG3** will is currently in transition, with prior efforts in charge and spin transport in quasi-1D nanostructures, using single-crystal nanowires grown by electrochemical, CVD methods and fiber deposition at extreme aspect ratios transitioning to a new effort in ordered three-dimensional metalattices formed by high-pressure chemical fluid deposition into ordered templates. This new effort exploits unique synthetic capabilities developed in the MRSEC and couples to unique high-harmonic coherent x-ray characterization techniques being brought into the MRSEC.

**IRG4** is also refocussing from a prior combination of in-fiber and planar nanostructured devices that manipulate and channel electromagnetic radiation across the spectrum into an effort focussed on assembly of complex, functional nanoparticle arrays with controlled degree of order and disorder for novel applications based on collective function, including coupled oscillator arrays, disordered photonics, and gradient optics. This effort exploits strong particle synthetic capabilities (including optical modulation of particle polarizability and design of “assembly-ready” hybrid particles with specific optical functionality) with innovative assembly methodologies, and takes advantage of capabilities in electromagnetic design developed in the prior instantiation of the IRG.

The seed grant program continue to be an important avenue for promoting new research ideas, particularly high-risk projects proposed by both early-career and established faculty, as described earlier. A strong matching commitment from Penn State allows the Center to support several seed projects in each annual competition. Historically, the seed program has been an important engine of innovation in the Center; for example, it led to the establishment of a new IRG (now IRG1) in the prior renewal. In 2013, the Center refocussed the “Seed IRG” on defects in 2D materials into a tight focus on novel 2D magnetic systems.

**Metrics:** The Center’s metrics for success include the number of collaborative publications, particularly those in high-profile journals and with multi-point collaboration, the degrees, training, outcomes and further career development of a diverse body of participants, numbers of patents, development of industrial and international collaborations, industrial co-sponsorship of research, and transfer of technology developed in the Center.

**Educational and Diversity Goals:** The Center maximizes its educational impact by coupling the expertise and enthusiasm of all of its members with our partners' expertise in reaching large
audiences. The *Science-U* summer camps, offered across grades 3–11, will continue to develop content on topics that resonate with the public. In partnership with The Franklin Institute (TFI), new museum shows will be created for distribution to a national network of science museums, reaching an audience of hundreds of thousands. We are recruiting at the high school level students both locally and from underrepresented groups in the Philadelphia area for a *Science Leadership* summer camp. A broad range of high schools and middle schools are being reached through teacher training workshops and research experiences, and a diverse group of students are mentored in the REU program, recruited through partnerships with minority-serving institutions. All major outreach programs are regularly assessed for efficacy and impact. Center outreach activities will continue to be integrated into the Center’s ongoing research activities through outreach showcases embedded into the MRSEC seminar series, participation across all levels in education and outreach activities, and the involvement of outreach staff in regular IRG research meetings and activities. In a new initiative, the MRSEC has sparked the creation of a STEM Open House, first offered in Fall 2013, as a means to facilitate the entry of undergraduates from underrepresented groups into graduate-level research. MRSEC also hosts Millennium Scholar undergraduate researchers in our labs, and will provide opportunities and support for these students through their entire undergraduate career.

The Center recruits students and postdocs from under-represented groups through ongoing collaborations with partner institutions in Puerto Rico, through the MRSEC facilities network, and by cultivating faculty contacts with minority-serving institutions. Our overriding goals are to nucleate institutional change through new programs such as the STEM Open House, and to consistently exceed minority representation in member departments. By coordinating with diversity-focused recruiting efforts across the campus through our Diversity Committee, the Center serves as a model and an agent for positive change in developing a diverse, interdisciplinary scientific workforce.
IRG1: Strain-enabled Multiferroics

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Overall Goal: This IRG broadly focuses on strain tuning and the resulting new phenomena in multiferroic materials in which two or more ferroic (ferroelectric, ferroelastic, magnetic) order parameters exist within a single material. The IRG in particular focuses on complex oxides, and the strain tuning is imparted in thin films of high crystalline perfection and precisely controlled strain state by appropriate choice of substrates and growth conditions through conventional and laser-based molecular beam epitaxy methods. The team’s expertise spans first principles and phase-field modeling predictions of new materials and phenomena, synthesis, structural electrical, magnetic, and optical characterization, and prototype device demonstrations.

Summary of Accomplishments: Of the six known mechanisms to create multiferroics, four of them have been proposed and discovered by this team. New ferroic phenomena in layered structures, domain walls and interfaces have been discovered. A new symmetry in nature (roto symmetry) has been discovered. Starting from its inception as a seed in 2006-2007, this group has published 166 peer-reviewed papers. This includes 12 in Nature and sister journals, 4 in Science, 15 in Phys. Rev. Lett. and others in journals such as Phys. Rev. B, Advanced Materials, Annual Review of Condensed Matter Physics, J. Am. Chem. Soc., Adv. Mater., Appl. Phys. Lett., J. Appl. Phys., etc. Over 50% of these publications involve at least two MRSEC PIs. The team has graduated 13 PhDs and 5 postdocs.

IRG RESEARCH HIGHLIGHTS:

Jahn-Teller distortion and Dzyaloshinsky-Moriya interaction, and hybrid improper multiferroicity.


- Discovery of thermotropic phase boundaries in classic lead-free ferroelectrics, such as BaTiO$_3$ and KNbO$_3$ in analogy with morphotropic phase boundaries in lead-based ferroelectrics. Similar low symmetry phases are predicted in multiferroics (Phys. Rev. B, 2013).

- A paraelectric antiferromagnet in bulk form such as EuTiO$_3$, when biaxially strained in thin film form becomes a strong ferroelectric ferromagnet. Electric-field control of magnetic interactions have been demonstrated (Nat. Comm. 2013). Landau theory for electric control of ferromagnetic phase has been developed (Phys. Rev. B, 2014).


- Discovery of flexo-roto effect involving coupling between strain gradients and octahedral rotations at domain walls and surfaces (Phys. Rev. B). Quantitative mapping of octahedral rotations in perovskite oxides.


**HIGHLIGHTS FROM 2013-2014:**

Discovering Thermotropic Phase Boundaries in Classic Ferroelectrics (Nature Commun. 2014): High performance piezoelectrics are lead-based solid-solutions that exhibit a so-called morphotropic phase boundary, which separates two competing phases as a function of chemical...
composition; as a consequence, an intermediate low-symmetry phase with a strong piezoelectric effect arises. In search for environmentally sustainable lead-free alternatives that exhibit analogous characteristics, we use a network of competing domains to create similar conditions across thermal inter-ferroelectric transitions in simple, lead-free ferroelectrics such as BaTiO$_3$ and KNbO$_3$. Here we report the experimental observation of *thermotropic* phase boundaries in these classic ferroelectrics, through direct imaging of low-symmetry intermediate phases that exhibit large enhancements in the existing nonlinear optical (Fig. 1) and piezoelectric property coefficients. Furthermore, the symmetry lowering in these phases allows for new property coefficients that exceed all the existing coefficients in both parent phases. Our findings reveal that phase transitions in ferroelectrics are intimately coupled to the underlying domain microstructure. Even in lead-free BaTiO$_3$ and KNbO$_3$, classic materials that have been known and studied for over sixty years, we have discovered that domains can lend a thermotropic character to their otherwise well-known phase transitions. This leads to the emergence of intermediate monoclinic phases in a wide temperature range around the conventional ferroelectric transitions. As this phenomenon arises due to the mechanical and dipolar interactions between competing ferroelectric-ferroelastic domains in a complex domain microstructure, advanced nanoscale-resolved multi-technique measurements in the same spatial location, such as those presented here, are required to properly reveal the underlying physics on a microscopic level. We show that in the stabilized intermediate phases, both the piezoelectric and the nonlinear optical properties can be strongly enhanced, and even newly induced. Since the mechanism of symmetry lowering through stresses and fields is in principle universal to non-triclinic ferroelectric crystal systems, these results suggest a host of possibilities for the design of high-performance phases. A fourfold (4×) enhancement in functional coefficients from a simple shear strain on the order of $10^{-4}$ indicates that controlled symmetry lowering can indeed be a powerful tool for property enhancement and tuning, and that it does not necessarily require large strains. In this study, a random domain microstructure was shown to inherently generate such strains, thus stabilizing the monoclinic phase. Theory however shows that similar shear stresses and fields, when applied externally to a single domain system, can also generate such monoclinic phases, along with the concomitant property enhancements. Moreover, since symmetry allows the ferroelectric

![Fig. 1. Local symmetry imaging and analysis by optical Second Harmonic Generation.](image)

Scanning SHG microscopy image of an in-plane a,b-domain structure in a BaTiO$_3$ single crystal a, without orthogonal twinning. Scale bar is 8 μm, and b, with orthogonal twinning. Scale bar is 12 μm. c, SHG intensity polar plots versus fundamental polarization angle (azimuth angle θ) corresponding to the $M_C$ phase. Data points are experiments, and the solid lines are theory based on a monoclinic $m$ point group symmetry. d, For tetragonal domains ($4mm$ symmetry), only the tensor coefficients without superscript (in black) are nonzero. For monoclinic $m$ symmetry ($m$ in-plane), the tensor coefficients with superscript $m$ (in red) also become nonzero.
polarization to lie anywhere within the monoclinic mirror plane, \( m \), it is easy to reorient the local polarizations in a polydomain monoclinic system with external fields to achieve a “poled” monoclinic domain microstructure. In addition, the piezoelectric tensor of the monoclinic phase enables shear modes that are particularly suitable for shear mode piezoelectric devices. Capturing these phenomena using phase field theory opens the door to predictive modeling of enhanced material properties, and enables the optimization of relevant extrinsic factors such as domain distribution, impurity content, and external fields. The fundamental insights presented in this work will allow for further exploration of strategies to reliably and reproducibly create these high-performance phases through ‘domain-engineering-by-design.’

**Exploiting Dimensionality and Defect Mitigation to Create Tunable Microwave Dielectrics** (*Nature*, 2013)

The miniaturization and integration of frequency-agile microwave circuits—electronically-tunable filters, resonators, phase shifters and more—with microelectronics offers tantalizing device possibilities, yet requires thin films whose dielectric constant at GHz frequencies can be tuned by applying a quasi-static electric field. Appropriate systems, e.g., \( \text{Ba}_n\text{Sr}_{1-n}\text{TiO}_3 \), have a paraelectric-to-ferroelectric transition just below ambient temperature, providing high tunability. Unfortunately such films suffer significant losses arising from defects. Recognizing that progress is stymied by dielectric loss, we start with a system with exceptionally low loss—\( \text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1} \) phases—where (SrO) planes provide an alternative to point defect formation for accommodating non-stoichiometry. These Randlesden-Popper (RP) layered phases (Fig. 2), given by the general formulae \( A_{n+1}B_n\text{O}_{3n+1} \), can be considered as alternating layers of perovskites (\( \text{ABO}_3 \)) and rock salt (AO), given by the sequence, \( n(\text{ABO}_3)/\text{AO} \). Our team has predicted from first principles calculations, an unusual polar state in the low \( n \), \( \text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1} \), at small values of tensile strain, in which ferroelectricity is nearly degenerate with true anti-ferroelectricity, a relatively rare form of ferroic order. With increasing \( n \) at a fixed value of epitaxial strain, a region of the phase diagram is reached where ferroelectricity and anti-ferroelectricity compete. Beyond a critical \( n>n_c \), an in-plane polarization sets in within the perovskite layers. This indicates the importance of the dimensionality “\( n \)” in turning on and off the ferroelectric properties of the series. We have observed the highest figure of merit for high frequency (GHz) dielectric tuning (% tunability divided by tangent loss) in these RP-phases. We report the experimental realization of a highly tunable ground state arising from the emergence of a local ferroelectric instability in biaxially strained \( \text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1} \) phases with \( n \geq 3 \) at frequencies up to 120 GHz. In contrast to traditional methods of modifying ferroelectrics—doping or strain—in this rather unique system increasing the separation between the (SrO) planes bolsters the local ferroelectric instability. This new control parameter, \( n \), can be

![Fig. 2: Ferroelectric Randlesden-Popper \( \text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1} \): Schematic of the crystal structure of a unit cell of the \( n = 1–6 \), and \( \infty \) members of the \( \text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1} \) phases. \( Q \) and FOM of the \( n = 6 \) sample at a bias field of 50 kV/cm, along with the room temperature FOM of a \( \text{Ba}_n\text{Sr}_{1-n}\text{TiO}_3 \) film at 300 kV/cm. The FOM of the \( n = 6 \) sample assumes that the loss tangent depends linearly on frequency and that the tunability is independent of frequency and 20% at a bias of 50 kV/cm. Solid points are \( Q \)-values averaged over a frequency range of 14.5 GHz.](image-url)
exploited to achieve a figure of merit at room temperature that surpasses all known tunable microwave dielectrics.\(^{48}\)

**Atomic Scale Mechanisms of Ferroelectric Switching** *Nature Commun.*, 2013\(^{47}\):

Polarization switching in ferroelectric thin films occurs via nucleation and growth of 180° domains through a highly inhomogeneous process in which the kinetics are largely controlled by defects, interfaces and pre-existing domain walls. We performed the first real-time, atomic-scale observations and phase-field simulations of domain switching dominated by pre-existing, but immobile, ferroelastic domains in Pb(Zr\(_{0.2}\)Ti\(_{0.8}\))O\(_3\) thin films. Our observations revealed a novel hindering effect, which occurs via the formation of a transient layer with a thickness of several unit cells at an otherwise charged interface between a ferroelastic domain and a switched domain. This transient layer possesses a low-magnitude polarization, with a dipole glass structure, resembling the dead layer. The study provides an atomic level explanation of the hindering of ferroelectric domain motion by ferroelastic domains. Hindering can be overcome either by applying a higher bias or by removing the as-grown ferroelastic domains in fabricated nanostructures.

**Quantitative Determination of Octahedral Rotations** *Phys. Rev. B*, 2013\(^{39}\):

In recent years, there has been an increased interest in octahedral rotations in perovskite materials, particularly on their response to strain in epitaxial thin films. The current theoretical framework assumes that rotations are affected primarily through the change in the in-plane lattice parameters imposed by coherent heteroepitaxy on a substrate of different lattice constant. This assumption has not been tested quantitatively over a range of strain states. To assess the validity of this picture, coherent LaAlO\(_3\) thin films were grown on SrTiO\(_3\), NdGaO\(_3\), LaSrAlO\(_4\), NdAlO\(_3\), and YAlO\(_3\) substrates to achieve strain states ranging from +3.03% to −2.35%. The out-of-plane and in-plane octahedral rotation angles were extracted from the intensity of superlattice reflections measured using synchrotron x-ray diffraction. The measured rotation angles were compared with those calculated previously for defect-free films. Good
agreement between theory$^{53}$ and experiment was found, suggesting that the current framework correctly captures the appropriate physics in LaAlO$_3$.

REFERENCES


IRG 2: Powered Motion at the Nanoscale

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Efficiency of Nano/micromotors: In the decade since our first paper on catalytic nanomotors (Paxton et al., J. Am. Chem. Soc. 2004, 126, 13424) appeared, a number of different propulsion mechanisms have been demonstrated for autonomous nano- and micromotors. Chemical propulsion has been observed deep in the nanoscale regime, at the level of individual enzyme and catalyst molecules. We have conducted a combined experimental and computational study (Wang et al. J. Am. Chem. Soc. 2013, 135, 10557) that quantifies the four stages of energy loss for self-electrophoretic catalytic motors as a function of length scale and chemical reaction type. Although the efficiency of H$_2$O$_2$-powered bimetallic rod motors is low ($\sim$10$^{-9}$), it can be increased approximately 1000-fold by using bipolar reactions that occur selectively at the anode and cathode segments of rods, and by designing annular motors that inhibit diffusion of the reaction products, thereby maintaining a larger chemical gradient. Interestingly, theory suggests that self-electrophoretic Janus particle motors may become more efficient on the sub-micron length scale. These studies show that bubble-powered and thermophoretic motors are inherently inefficient on the micron length scale, but that magnetically propelled helical micromotors and acoustically propelled motors can be much more efficient (Table 1).

**Table 1:** Comparison of the energy efficiencies ($\eta$) of different types of micromotors.

<table>
<thead>
<tr>
<th>Motor Type</th>
<th>Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Macroscopic electric motor</td>
<td>0.8</td>
</tr>
<tr>
<td>Kinesin molecular motor</td>
<td>0.6</td>
</tr>
<tr>
<td>Flagellar bacterium</td>
<td>0.02</td>
</tr>
<tr>
<td>Helical magnetic micromotor</td>
<td>$10^{-7}$ - $10^{-3}$</td>
</tr>
<tr>
<td>Self-electrophoretic Janus motor</td>
<td>$10^{-6}$ - $10^{-1}$</td>
</tr>
<tr>
<td>Acoustic microswimmer</td>
<td>$10^{-7}$</td>
</tr>
<tr>
<td>Bubble-powered micromotor</td>
<td>$10^{-9}$ - $10^{-10}$</td>
</tr>
<tr>
<td>Thermophoretic micromotor</td>
<td>$10^{-13}$</td>
</tr>
</tbody>
</table>

Dynamic Interactions of Self-electrophoretic Micromotors: One of the challenges in the design of colloidal active matter is understanding the pairwise forces that develop between...
powered particles. We have used observations of the chemically powered assembly of bimetallic nanorods (Fig. 1) to quantify the catalytically generated electrical forces between pairs of rods and between rods and passive tracer particles. (Wang et al., *PNAS* 2013, 110, 17744). The catalytic decomposition of H$_2$O$_2$ generates protons at the anode ends of the rods, resulting in a dipolar charge distribution. Rods moving in the same direction form staggered doublets and triplets to minimize the local electrostatic energy. The dissociation of these doublets and triplets follows an Arrhenius rate law, from which the dissociation energy was calculated. By measuring the speed of tracer particle approach to the nanorods as a function of distance, we were also able to calculate the force-distance relationship using the Stokes law. These observations provide us with a complete energetic description of powered assembly in the system of bimetallic nanorods and passive tracer particles. The forces and energies of these interactions can be used as inputs to atomistic models of colloidal assembly, which gives rise to emergent collective behavior in systems of powered microswimmers. We plan to work with collaborator Ramin Golestanian on the mapping of phase diagrams of collective behavior based on these interactions.

**Acoustic propulsion of autonomous micromotors:** Following up on our discovery, reported last year, of a new acoustic propulsion mechanism for nanorod motors, we have studied the propulsion mechanism and have also investigated the interaction of the motors with living cells. We fabricated Au cones and flat arrows on length scales of 1-20 µm, both by electrochemical replication of alumina templates and by projection lithography. In each case, the objects had one concave end, and were studied using resonant ultrasound (~4 MHz) that levitated them to the midpoint of a cylindrical observation cell in water. For the largest of the objects, the motion was dominated by the acoustic radiation force and they were rapidly driven to the acoustic nodes in xy plane of the cell. The smaller objects were propelled axially, but the flat arrows tended to move towards the concave end, in contrast to the behavior found with electrochemically grown rods. This suggests that the axial propulsion we observe for metal rods may arise more from material asymmetry than from shape asymmetry. We are currently studying bimetallic rods made from a variety of different metals to test this hypothesis.

By adding ferromagnetic nickel stripes to the midpoints or ends of metallic nanorods, we are able to orient acoustically propelled motors in weak magnetic fields (Ahmed et al., *Langmuir* 2013, 29, 16113), and we have also observed the assembly of magnetic rod dimers, trimers, tetramers, and higher aggregates, all of which can be powered acoustically. When Au or bimetallic AuRu rods are incubated with live HeLa cells, they adhere to the outer leaflet of the cell membrane.
Over a period of 24 h the cells ingest the rods, apparently by phagocytosis (Fig. 2). The rods are mobile inside the cells and can be propelled in the acoustic observation cell for several minutes without adversely affecting the viability of the cells. Both axial translation and spinning can be powered inside the cells (Wang et al., Angew. Chem., in press). Tracking of rod movement inside the cells shows very rapid re-orientation relative to movement in water. This is consistent with the crowded and structured environment of the cell interior. Interestingly, local mechanical excitation of intracellular organelles (most likely the endoplasmic reticulum) causes movement of organelles in other parts of the cells. At this point it is unknown if this arises from mechanical or chemical communication between these remote parts of the cell.

**Selectively Manipulable Acoustic-powered Microswimmers:** The physics governing swimming at the microscale—where viscous forces dominate over inertial—is distinctly different than that at the macroscale. But if we can master these physics and create devices capable of finely controlled swimming at the microscale, we can enable bold ideas such as targeted drug delivery, non-invasive microsurgery, and highly precise materials assembly. Some progress has already been made towards such artificial microswimmers, using various means of actuation: chemical reaction, diffusion-driven, self-thermophoresis, applied magnetic, electric, and acoustic field. However, the prevailing goal of selective actuation of a single microswimmer from within a group—the first step towards collaborative action by a group of swimmers—has so far not been achieved. In this letter, we present a new class of microswimmer, accomplishing for the first time selective actuation. Our swimmer design eschews the commonly-held design paradigm that microswimmers must use non-reciprocal motion to achieve propulsion; instead, the swimmer is propelled by oscillatory motion of an air bubble trapped within the swimmer’s polymer body. This oscillatory motion is driven by application of a low-power acoustic field, which is biocompatible to cells and other biological samples, to the ambient liquid, with meaningful swimmer propulsion occurring only at resonance frequencies of the bubble. This acoustically-powered microswimmer (Fig. 3) accomplishes controllable and rapid translational
and rotational motion, even in highly viscous liquid. And by using a group of swimmers each with a different bubble size—leading to different resonance frequencies—selective actuation of a single swimmer from among the group can be readily achieved.

**Fig. 3.** Selective actuation of a swimmer from within a group. Two swimmers, each with a bubble of different size, were exposed to the same acoustic field, and a frequency sweep was performed. a. Swimmer A starts to move substantially at an excitation frequency of 74 kHz, with minimal motion of swimmer B (see also Supplementary Video 7). b. The frequency is then gradually increased, stopping movement of swimmer A. At an excitation frequency of 91 kHz, swimmer B starts to move while swimmer A remains stationary.

The IRG has developed an efficient and parsimonious matrix-based theory for studying the ensemble behavior of nanomotors (and other autonomous propellers), systems that are typically studied by much more cumbersome differential-equation-based Langevin or Fokker-Planck formalisms. The kinematic effects for elementary processes of motion are incorporated into a matrix, called the “kinematrix”, from which one can immediately obtain correlators and the mean and variance of angular and position variables (and thus effective diffusivity) by simple matrix algebra. The kinematrix formalism enables the behaviors of a diverse range of self-propellers to be recast into a unified form, revealing universalities in their ensemble behavior in terms of new emergent time scales. For example, this formalism can describe how the coupling of rotation to orientational diffusion yields chiral translational diffusion which can dominate the ordinary thermal translational diffusion for experimentally relevant nanomotors. Unpowered chiral particles do not exhibit chiral diffusion, but a nanorotor has both handedness and an instantaneous direction of powered motion, thus -- unlike an unpowered particle -- its diffusional motion can distinguish left from right. Effort to experimentally observe this chiral diffusion are in progress. Further theory advances provide insights into the distribution of motive force across the surface of the nanomotor. For a given motor type, the underlying chemical reaction that enables motility may be clear, but the quantitative mechanism by which this reaction breaks symmetry and converts chemical energy to mechanical motion is often less clear, since it is difficult experimentally to measure the spatial distribution of chemical species around the nanorotor during operation. We have demonstrated how the experimental trajectory of a nanorotor can provide quantitative information about the role of asymmetry in nanomotor
operation and provide insights into the spatial distribution of motive force along the surface of the nanomotors studied in the IRG. At a more detailed mechanistic level, the IRG has developed a general analysis connecting flux-based and kinetics-based analyses of the electrokinetic locomotion of spherical electrocatalytic nanomotors, in the linear regime, using the method of matched asymptotic expansions. Flux-based approaches require a distribution of cation flux over the nanomotor surface as an input, while kinetics-based approaches start from redox kinetics for production and consumption of ions. Employing a general flux-based approach, we obtain a universal expression for nanomotor velocity to leading order in Debye length and surface cation flux for spherical motors, and then demonstrate how to match that calculation to a general Butler-Volmer model for electrochemical redox kinetics, obtaining an expression for motor speed in terms of inhomogeneity of rate coefficients. To expose an underlying physical picture and connect the rigorous calculations to intuition, we also give a scaling analysis based on straightforward physical reasoning.

**Enzymes as Molecular Motors and Pumps:** We have shown, for the first time, that single enzyme molecules can generate sufficient mechanical force through substrate turnover to cause their own movement and, more significantly, the movement becomes directional through the imposition of a gradient in substrate concentration, a form of chemotaxis at the molecular level (Sengupta et al., *J. Am. Chem. Soc.* 2013, 135, 1406). Further, this results in chemically interconnected enzymes being drawn together; a primitive form of predator-prey behavior. The findings allow the design of “intelligent,” enzyme-powered, autonomous nano- and micromotors, with possible applications in pattern formation, drug delivery at specific locations, roving sensors, and separation of catalyst molecules based on activity.

When anchored on a surface, the same enzymes transfer their chemically-generated force to the surrounding fluid; in effect, immobilized enzyme systems can be used as micropumps in the presence of their specific substrates or cofactors (Fig. 4) (Sengupta et al., *Nature Chem.* 2014, *in press*). This discovery enables the design of non-mechanical, self-powered nano/microscale pumps that precisely control flow rate and turn on and off in response to specific analytes. The recent experiments establish three important findings: 1) Essentially all surface-anchored enzymes act as pumps when turning over their substrates, 2) these pumps are selective for the substrate of a particular enzyme, and 3) neighboring pumps interact through fluid convection loops and diffusive transport of solutes and particles. Enzyme promoters or cofactors can also trigger and regulate pumping. Similar pumping can occur in gel particles in which the enzymes are immobilized. For example, bound glucose oxidase pumps insulin out of gel particles when glucose is added to solution.
Self-Powered Polymeric Pumps with Memory: We recently developed small molecule reagents that can be grafted onto polymer beads or surfaces to create a variety of smart pumps (Angew. Chem. Int. Ed. 2013, 52, 10295). One example is shown in Fig. 5; here, a 300 µm-diameter polymer bead was modified with two reagents. One of the reagents responds to UV light (which is the stimulus in this case) and releases multiple copies of a small molecule signal transduction reagent (e.g., fluoride). The signal transduction reagent then reacts with the second reagent on the bead, which supports a self-propagating reaction by consuming itself. Both reactions release additional small molecule products that diffuse away from the bead and, thus, cause the surrounding fluid to move (the bead is now a pump). The bead pumps the fluid when exposed to the UV light, but it also pumps the fluid when the UV light is removed—the self-propagating reaction keeps the pump operating once the stimulus is removed. In the absence of the stimulus, the pump remains off. Thus, the bead (pump) has a “memory” for the stimulus and is capable of responding even when the stimulus is fleeting. An attractive feature of this type of system is the ease with which we should be able to modify the chemistry of the reagents to enable the system to respond selectively to a variety of stimuli.

Fig. 4: (a) Enzyme-powered pump. Au patterned on PEG-coated glass is functionalized with quaternary ammonium thiol that binds enzyme molecules. Local fluid pumping is initiated by addition of the appropriate substrate(s). (b) Multi-enzyme cascades can be patterned on a chip to enable positive and negative feedback, regulation and microfluidic logic. In this example, the reaction of glucose at glucose oxidase pump generates H$_2$O$_2$, which actuates a catalase pump.
We also developed a second type of smart pump based on polymers that depolymerize from head-to-tail when specific functionality (i.e., an end cap) is cleaved from the terminus of the polymer in response to a specific signal. We reported on this type of pump previously (Angew. Chem. Int. Ed. 2012, 51, 2400), but now we have studied the effect of the polarity of the end cap on the accessibility of the end cap to an analyte in solution at the solid-liquid interface. This new study (Macromolecules 2013, 46, 7257) has enabled the smart pumps to respond to analytes substantially faster than was previously possible. Our work on smart pumps with a “memory” provides a new capability to the area of nanomotors/pumps and offers the opportunity for amplified responses as well as sustained responses to specific applied signals. Our future efforts will seek to expand this type of chemistry that enables continuous responses in solid materials.

Moving forward, we hope to achieve a hierarchical understanding of the dissipative behavior of active matter from the level of individual active molecules, such as enzymes, up to assemblies of nano/micromotors and pumps. This knowledge will be specific, encompassing the details of individual motility mechanisms, yet generic, by way of guiding principles, symmetry properties, and effective theories describing the coarse-grained collective behavior of non-equilibrium systems. The proposed work will lead to the formulation of overall phase diagrams, which will allow us to engineer systems from the single particle level for the desired collective behavior as an emergent property. Practical systems applications, which are already beginning to emerge from this work, will exploit the team’s combined ability to synthesize, test, and model motors and pumps driven by a number of interacting propulsion mechanisms. Ultimately, broad new capabilities in the design of active matter should result from this research.
IRG3: Electrons in confined geometry

Faculty Participants: Moses Chan (leader), John Badding, Jainendra Jain, Qi Li, Chaoxing Liu, Suzanne Mohney, Joan Redwing, Nitin Samarth, Srinivas Tadagadapa
2 post-docs and 7 graduate students

The theme of this IRG is the study of the physics of superconducting, metallic, magnetic and semiconducting nanowires in the 1D limit. We will summarize below the progress we have made during the past year on a number of projects.

Superconductivity and single-fluxon controlled resistance switching in centimeter long Ga-In nanowire: We have made substantial progress in understanding the transport properties of centimeter length Ga and Ga-In nanowires of 150 nm diameter. These wires were fabricated by high pressure infiltration into silica capillary with a hollow inner diameter of 150 nm when the metals are in the liquid phase. Most of the capillaries used in our studies are provided by colleagues at the University of Southampton. We have also begun fabricating glass fibers at Penn State with smaller inner diameters using a Vytran GPX-2400 glass fiber processor in the past year. SEM and AFM investigations reveal that diameters of these capillaries vary by less than 1 nm over centimeters of length, with surface roughness on the order of +/-0.1 nm RMS. Electrical contacts to a 6 mm segment of the wires are made by immersing both ends into millimeter size droplets of Ga or Ga-In (Fig.1c).

Fig. 1. a, An optical image of the glass fiber infiltrated with Ga. b, An end view of a hollow fiber by field emission SEM. c, The schematic for four probe transport measurements. d, R vs. T at zero field of pure Ga wire showing a superconducting transition at 1.1 K, the bulk Tc value. The inset shows a warming-cooling hysteresis loop, indicating that Ga inside the fiber freezes at 250 K instead of 303 K, the bulk freezing point. e, R vs. T scan at zero field for a Ga-In nanowire. A two stage superconducting transition at 3.5~5 K and 1.1 K is found. Warming and cooling hysteresis similar to that of pure Ga is also found.

Fig. 1d show resistance (R) vs. T results on a pure Ga wire of 150 nm. The resistivity of the solid 150 nm Ga wire at 250 K (see figure caption) is on the same order as the bulk Ga crystal. The tenfold drop in resistance from 250K to 4K (Fig 1d) indicates that our nanowires are of much higher quality than those fabricated by e-beam assisted evaporation. A sharp drop in R from 11kΩ down to 0.1 Ω, the resolution of our measurement with an excitation current of 5 nA is found at 1.1K, the superconducting transition of pure bulk Ga. It appears the wire is not yet in the 1D limit. Measurements will be made on wires of smaller diameters.

Fig.1e shows zero field R vs. T results of a Ga-In wire at a Ga concentration that is slightly above the eutectic concentration (75% Ga by weight). The R vs. T plot exhibits a two-step transition: from 12 kΩ to 60 Ω between 3.5 and 5 K, and then to the zero resistance superconducting state at 1.1 K, the Tc of bulk Ga. This can be understood in terms of phase separation into two regions; one is the pure Ga with a lower superconducting transition (Tc) at 1.1 K which separates first, and
the other containing Ga-In eutectic (EGaIn) with a higher superconducting transition ($T_c'$) at 3.5–5 K.

The magneto-resistance (MR) results are qualitatively different below and above $T_c = 1.1$ K. At $T = 1.2$ K, the MR stays constant at 60 $\Omega$ at low field and increases with magnetic field for $H > 500$ Oe which plateaus to the normal state value of 11 k$\Omega$ near 2800 Oe when the GaIn wire becomes normal (Fig.2c) The MR below 1.1K (Fig. 2a, b) show novel hysteretic jumps between zero to 60 $\Omega$. When the magnetic field ($H$) is increased to a specific value, which we designate as $H_{c1}$, the resistance ($R$) abruptly jumps from zero to 60 $\Omega$ and stays at this value even when $H$ is reversed back to zero. When $H$ reaches a negative critical field ($-H_{c1}$) ($|H_{c1}| < |H_{c1}|$), $R$ drops back to zero. $R$ jumps up to 60 $\Omega$ again when $H$ reaches $-H_{c1}$. After $H$ reverts back to positive direction, $R$ will follow a symmetric loop. Hysteretic behavior was also seen in $R$ vs. $T$ scans at fixed $H$ above a certain value. Fig. 1d,e show $R$ vs. $T$ scans undergoing a warming-cooling cycle from 0.5 to 8 K under 0 and 200 Oe, respectively.

![Fig. 2. a,b,c, Magnetoresistance (MR) measurements of the GaIn wire at 0.5 K, 1.0 K and 1.2 K. d,e, R vs. T scans at 0 Oe and 200 Oe. Hysteresis is found at 200 but not at 0 Oe. All MR scans began by cooling the sample from 8K to 0.5K under zero magnetic field.](image)

The 60 $\Omega$ resistance jump is undoubtedly the consequence of flux trapping in the wire that drives a fraction of the wire ‘normal’. A microscopic model that is consistent with all the experimental observations calls for the phase separated residual pure Ga forms nanodroplets that are surrounded by EGaIn. The existence of such Ga nanodroplets is confirmed by X-ray fluorescence spectroscopy studies carried out by us at the Advanced Photon Source at the Argonne National Laboratory (Fig. 3a). Our model posits a pair of Ga nanodroplets that are in close proximity with each other. The smaller Ga nanodroplet is surrounded by a sufficiently thick EGaIn shell that makes it possible to trap 1 or 2 fluxons when EGaIn is superconducting. The
diameter of the larger Ga limits the thickness of the surrounding EGaIn and prevents the trapping of even 1 fluxon. However, it creates a Josephson weak-link out of the surrounding thin GaIn shell. When the larger Ga nanodroplet is superconducting, the system shows zero resistance. 60 Ω appears when the larger Ga nanodroplet is driven normal by one trapped fluxon with additional external magnetic or by two trapped fluxons in the smaller nanodroplet at zero or low magnetic field. This experiment shows that we can induce the switching between a resistive and a non-resistive state in a cm long quasi 1D superconducting Ga-In nanowire by the addition of a single flux quantum. We note that the quasi-1D geometry is crucial for this purpose; in two or three dimensions, a single fluxon does not cause a macroscopic step change in the resistance. The long length of the wire is also important, because the effect depends on a relatively rare configuration of a pair of Ga nanodroplets in close proximity with each other. The results reported here will be submitted for publication soon.

**Observation of individual macroscopic quantum tunneling events in aluminum nanowires:**

In quasi one dimensional (1D) nanowires, superconductivity is destroyed by phase slip events. Phase slips can be caused by thermal activation over a free energy barrier (TAPS) or quantum tunnelling through the barrier (QPS). QPS is an example of macroscopic quantum tunnelling. It is a challenge to cleanly differentiating between QPS and classical TAPS events in nanowires. We have made use of a phenomenon discovered in 2005 by this IRG known as the antiproximity effect (APE) to experimentally separate QPS from interference of TAPS in aluminium nanowires. In APE a superconducting nanowire is driven normal when the electrodes are brought from the normal to the superconducting state. This phenomenon is a confirmation of the Caldeira-Leggett mechanism where the superconductivity of the nanowire is stabilized by the dissipative environment provided by the normal electrodes. When the electrodes are superconducting phase slips or quantum tunnelling becomes possible. Aluminium nanowire and aluminium electrodes were fabricated by e-beam assisted evaporation where the electrodes have superconducting transition temperature lower than that of the nanowire. In such a system, the high temperature TAPS dominated region of the nanowire is cleanly separated by a phase-slip free superconducting region stabilized by the normal electrodes from the low temperature region where QPS are observed. Individual QPS are detected in the nanowire by means of a novel single-shot voltage measurement protocol, in which they appear as stochastic switching events from the superconducting to the normal state. The results of this experiment was published in August, 2013 (Phys. Rev. B 88, 064511(2013))
Physical Mechanism for the Long Range Proximity Effect in Ferromagnetic Nanowires:

Three years ago we reported a long-range proximity effect (extending over ~500 nm) in ferromagnetic Co and Ni NWs. This is completely unexpected in view of the incompatible spin orders of ferromagnetism (spin polarized) and superconductivity (spin singlet).

In the experiment, polycrystalline Co and Ni NWs, grown by electro-deposition, were individually contacted by four superconducting W strips deposited using a focused ion beam (FIB). In addition to a substantial drop in resistance R at low temperature, we found a large peak in R immediately below T_c of the electrodes. Theoretical explanations of the observations include either modeling the W-Co-W or the W-Ni-W nanostructures as Josephson junctions, or, quite excitingly, induced triplet superconductivity in the ferromagnet. The large resistance peak near T_c of the superconducting electrodes can be understood as a consequence of a reduction in the density of states due to pairing fluctuations. We made transport measurements on Co NWs with only one superconducting (W) electrode and found comparable induced superconductivity, which rules out the Josephson junction interpretation. We have recently made measurements on Ni NWs, fabricated by e-beam assisted evaporation and contacted by Nb and Al electrodes (e-beam evaporation in the case of Al and sputtering in the case of Nb) [Fig.4]. The R vs T plot of the Ni wire contacted by Nb shows the same qualitative features as the crystalline Ni contacted by the W electrodes. The size of the effect with the Nb electrodes, as measured by the peak in R and the magnitude of the drop in R, is smaller. With Al electrodes, an even smaller peak is found, but there is no sign of a resistance drop down to 0.5 K. By estimating the spatial extent of the proximity effect via the drop in R normalized by the length of the Ni NW, we found 750 and 50 nm for the W and Nb electrodes, respectively. These features in R appear to show a trend that scales with the strength of the spin-orbit (SO) coupling of the three electrodes. These results are consistent with the interpretation that the induced superconductivity in the ferromagnetic is triplet and that SO coupling at the electrode/nanowire interface is responsible for “converting” the s-wave Cooper pairs to triplet pairs. Indeed, our recent theoretical work shows that while a ferromagnet converts singlet pairs into triplet pairs, SO coupling can be used to manipulate the “d-vector” of the triplet superconducting order. We will explore how to control the “d-vector” in the context of our specific experimental setups by numerical simulations of the “Usadel equation.”

Nanotubes of topological insulators and of systems with strong spin-orbit coupling:

Topological insulators (TIs) are insulating in bulk, but their surface contains conducting states with exotic physical properties. Recently, progress has been made towards

Fig 4 R vs. T scans at zero and finite magnetic fields of Ni nanowires contacted by FIB W (red, Ni nanowire is polycrystalline), e-beam Nb (blue) and e-beam Al (green) electrodes. The length of the wires between the voltage probes (L) are 3 (W), 2 (Nb) and 1 (Al) µm. Cross sections of the Ni wires are 60 x 60 (nm) (W), 50x100 (nm) (Nb) and 50x50 (nm) (Al). Normal state resistances are 186 Ω (W), 30.5 Ω (Nb) and 23.8 Ω (Al).

Fig 5 (a) Quantum oscillations in magnetoresistance of Bi_2Te_3 nanotubes observed at 1.8 K. The inset is a TEM image of one of the larger Bi_2Te_3 nanotubes. (b) Fitting of the resistance oscillation with two frequencies.
eliminating bulk conduction using either appropriate crystal engineering or electrical gates, although the carrier mobility remains limited. Alternate nanoscale geometries could suppress bulk transport further while also enhancing coherent quantum transport. We initiated an electrical transport study of TIs of Bi$_2$Te$_3$ nanotubes, a geometry that produces topological surface states with a confinement-induced gap. In contrast to the better-studied nanoribbons and NWs that are fundamentally similar to the bulk, such nanotubes have a unique real-space “doughnut” topology. In collaboration with colleagues at USTC of China, we have used a chemical solution phase method to synthesize crystalline Bi$_2$Te$_3$ nanotubes with a typical length of 10 µm, and inner and outer diameters in the range of 50-150 and 70-200 nm (Fig. 5a). Electrical transport measurements show a semiconducting behavior, in contrast to the mostly metallic behavior found in undoped/ungated bulk crystals and thin films. Quantum oscillations with two distinct frequencies in magneto-resistance are observed when a magnetic field is applied parallel to the nanotubes, with a main period around 4670 Oe, existing up to 9T, and a second period of 2560 Oe, decaying more rapidly with increasing field and dying off around 3T (Fig. 5b). The main (4670 Oe) periodicity originates from the anomalous Aharonov-Bohm (AB) effect, which is due to the surface state changing from gapped (at zero field) to gapless (enclosing field of half integer flux quantum). The second oscillation might be from either the Alshuler-Aronov-Spivak (AAS) effect or anomalous AB oscillations from the inner surface.

**Spin caloritronics at nanoscale:** The interplay of spin, charge and thermal transport in metals and semiconductors raises many unsolved fundamental puzzles such as the role of “magnon drag” in the thermoelectric properties of ferromagnetic metals to the origins of the recently discovered “spin Seebeck effect”. Experimental work in this rapidly developing field of “spin caloritronics” has largely focused on thin films and bulk crystals. We began this past year a program to explore spin caloritronics in an uncharted low-dimensional geometry, suspended nanowires and nanotubes, driven by the intuition that nanostructures provide relatively simple model geometries wherein both electronic, magnetic and (possibly) phonon degrees of freedom can be systematically and independently varied. Nanostructured ferromagnets also simplify the domain structure, thus removing the complexities created by multiple domain walls in more macroscale samples.

We have recently demonstrated proof-of-concept measurements of thermopower in Ni NW, Bi$_2$Te$_3$ nanotubes and GaAs/MnAs NWs (Figs. 6) in a microscale workbench. The GaAs/MnAs core shell NWs were grown by us by means of molecular beam epitaxy. Since the NWs are freely suspended between the two clamped ends, thermal cross-talk through the substrate is eliminated. Our long term goals are threefold: (1) definitively identify the role of magnon drag in thermoelectric properties of ferromagnetic NWs; (2) explore the role of critical fluctuations near a ferromagnetic phase transition on thermopower (the GaAs/MnAs NWs have a Curie temperature of 318 °C); (3) explore the effect of strong spin-orbit coupling and topological surface states (e.g. of the Bi$_2$Te$_3$ nanotube) on the spin caloritronic phenomena. Our proposed measurements range from fundamentally important (magnon drag in NWs) to technically challenging and transformative (spin Seebeck effect in NWs). We anticipate that the proposed projects will be influential within a burgeoning field where we hope to carry out the first spin caloritronic experiments in a single NW geometry.

![Fig. 6](image-url)
IRG 4: Electromagnetically Coupled Nanostructures

Faculty Participants: J. V. Badding, A. Borhan, V. Crespi, V. Gopalan, Z. Liu, T. S. Mayer, R. Schaak, D. H. Werner


This IRG has made significant progress in designing and fabricating in-fiber and planar nanostructured devices, which are being used to manipulate and channel electromagnetic (E-M) radiation across the spectrum. Semiconductors and metals have been integrated in the extreme-aspect ratio pores of microstructured optical fibers and new all-fiber optoelectronic and nanoscale imaging devices that exploit E-M coupling at dimensions down to the nanoscale and lengths up to meters are being developed. Genetically-inspired feed forward design methods are being used to create planar metallo- and all-dielectric nanostructures with user-defined E-M scattering. New passive and active (e.g., tunable) infrared and visible devices including wavelength-selective filters and mirrors, and entirely new materials with customized refractive indices including zero and negative index have also been realized.

Chemical Vapor Deposition Applied to other Geometries: Investigations of high pressure chemical vapor deposition (HPCVD) in optical fibers have revealed the mechanisms by which it is possible to deposit thin films conformally in constricted geometries. It now appears that HPCVD opens the possibility for deposition in many confined geometries other than optical fibers of considerable scientific and technological interest. For example, it is possible to deposit in planar geometries as long as one of the reactor dimensions is kept small enough (~10 to 100 µm) to preclude nucleation and growth of nanoparticles in the gas phase (Fig. 1). The technological potential for this approach is very large because it should allow for deposition over areas of hundreds of square meters of films of semiconductors such as hydrogenated amorphous silicon and crystalline silicon (Fig. 2). Furthermore, HPCVD is useful not only for planar

Fig. 1. (a) Schematic of high pressure CVD (HPCVD) in a macro-scale reactor. (b) SEM image showing Si particles dominate in the HPCVD process in macro-scale reactors (c) HPCVD in confined space. d) SEM image of smooth Si film deposited via confined HPCVD (left) and AFM topography image (right) showing 4 Å RMS roughness.

Fig. 2. Prototype HPCVD roll process. (a) Two stainless steel sheets of 50 µm thickness are partially overlapped and then coiled up together, with one serving as the spacer for the other (b) Roll of stainless steel sheet in a cylindrical chamber. (c) Sheet after deposition of a-Si:H film.
films, but also for “metalattices” (Fig. 3). The IRG has just recently begun work on these new ordered 3D geometries, as a major focus of activity in the future.

**Metalattices:** We define a metalattice as an artificial 3D solid that is periodic on a scale of 1-60 nm; depending on the detailed structure, it could be notionally subdivided into meta-atoms (e.g. more capacious regions that preferentially localize low-energy electronic states) linked by meta-bonds (e.g. thin channels that interconnect meta-atoms and facilitate dispersive states); Fig. 3 shows an example recently synthesized by HPCVD. In addition, an ordered, highly interconnected surface or interface interweaves the structure. A general means to synthesize ordered, 3D lattices with lattice constants of nm’s to 10’s of nm from a broad palette of materials could open up many opportunities for new physics when the structural order parameter of the lattice interacts with these intrinsic electronic, vibrational, optical, and magnetic processes in semiconductors, insulators, metals, and intimate co-lattices of two disparate such materials. We plan to investigate this physics.

Our work to date has been focused on synthesizing a wide range of metalattices to explore the lower size limits of infiltration by HPCVD and characterizing the properties of these materials. Even Vycor glass with a random network of 8 nm diameter pores can be infiltrated with Si to make a contiguous and photoluminescent network of semiconductor (Fig. 4). Thus electronic and photonic materials that combine both long-range electron transport and photoluminescence arising from quantum confinement can be synthesized. The properties of silicon can thus be altered for useful devices that emit light, for example. Photoconductivity experiments on amorphous silicon deposited within a silica optical fiber capillary and laser heated to crystallize it reveal that large bandgap shifts are possible as the amorphous silicon shrinks upon crystallization (Fig. 5.). Similarly, it is possible to infiltrated metalattice templates with amorphous silicon. It will be possible to laser crystallize to induce stresses that modeling indicates can be several GPa. These stresses should induce large and tunable shifts in the materials proper-

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**Fig. 3.** Metalattice Inverse Nano-Opal: (a) Infiltration of a semiconductor (purple) into a “nano-opal” template formed by close packed nm-scale silica spheres (green shells). (b) Transmission Electron Microscope (TEM) cross-section of a Si inverse nano-opal. Void-free infiltration of nano-opal templates this small with semiconductors has not been previously reported.

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**Fig. 4.** (a) Empty & intrinsic-Si infiltrated Vycor glass. (b,c) SEM of unfilled and filled pore (~4-7nm) network. (d) I-V curves of Vycor infiltrated with Si. Conductivity increases >1000x upon illumination, indicating that Si forms a conductive network.
ties of silicon. We will also investigate the synthesis of metalattices composed of compound semiconductors. The interplay of strain, 3D confinement, and interfaces across a range of semiconductor compositions promises rich physics and useful materials properties.

**Infrared High Resolution Imaging Fiberscopes**: Using a tapered Ge-infiltrated silica holey fiber array (Fig. 6), and treating each Ge fiber as a pixel to transmit infrared light, we have recently demonstrated infrared imaging spectroscopy. As an example, we have demonstrated that the different parts of a biological sample (e.g. fat versus muscle tissues) can be distinguished in an image by their different infrared absorption properties. This ability to perform sub-wavelength infrared spectroscopic imaging with the unique fibers can lead to biomedical applications in the future, such as infrared endoscopy.

**Non-linear Transmission Properties of Hydrogenated Amorphous Silicon Fibers**: HPCVD is unique in its ability to deposit low optical loss hydrogenated amorphous silicon in constricted geometries such as optical fiber pores. We have characterized the nonlinear Kerr effect and two-photon absorption of these fibers and found that the nonlinear figure of merit increases dramatically in the mid-infrared. They thus have good potential for non-linear applications in the mid-infrared.

**Ultrafast Optical Control Using Hydrogenated Amorphous Silicon Fibers Resonators**: Semiconductor microresonators allow for probing useful non-linear phenomena at low thresholds. We have characterized the size of the Kerr induced resonance wavelength shifting in a hydrogenated amorphous silicon fiber treated as a microcylindrical resonator. We have demonstrated its potential for ultrafast all-optical modulation and switching. Large wavelength shifts are observed for low pump powers due to the high non-linearity of the amorphous silicon material and strong mode confinement in the microcylindrical resonator. The threshold energy for switching is less than a pico-
Optical Metamaterials: This year we made significant progress in modeling, designing, and fabricating planar nanostructured devices to manipulate E-M radiation using genetically-inspired feed forward design methods. As a part of this effort we successfully designed, fabricated, and characterized optical electromagnetic bandgap (EBG) metamaterial coatings with near-perfect absorption over broadband ranges with greater than an octave of bandwidth and wide fields-of-view (FOV). The measured average absorption for the metamaterial in Fig. 7 is greater than 98% over a wide ±45° FOV for mid-infrared wavelengths between 1.77 and 4.81 µm. The nearly ideal absorption was realized by using a genetic algorithm (GA) to identify the geometry of a single-layer metal nanostructure array that excites multiple overlapping electric resonances with high optical loss across greater than an octave bandwidth. The response is optimized by substituting Pd for Au to increase the infrared metallic loss and by introducing a dielectric superstrate to suppress the reflection over the entire band.

We also developed a new class of ultrathin anisotropic metasurfaces composed of nanorod nanoantenna arrays for broadband and wide-angle polarization control and conversion. The versatility of this design approach was illustrated by demonstrating half-wave and full-wave plates that transform a linear incident wave to either a linear polarized wave or circularly polarized wave. A semi-analytical model was developed for fast evaluation of the performance of these metallodielectric nanostructures over a wide-FOV. Nanofabricated samples were characterized at different angles of incidence, showing polarization conversion ratios greater than 92% from 640 to 1290 nm over a wide FOV of ±40°, along with a power efficiency greater than 85% (Fig. 8). This work will enable ultrathin nanophotonic components with superior functionalities suitable for integration in practical optical systems.

Plasmonic Nanoparticles: In parallel with research on planar metamaterials and metasurfaces, we explored a variety of nanoparticle-based optical devices. We have studied the properties of layered plasmonic nanoparticles using spherical transmission line theory. This approach models the complex interaction of the nanoparticle with its surrounding as a combination of complex...
admittances. This allows the design of nanostructures with high-impedance or a high-admittance boundary conditions, which function as parallel and series LC resonators at the nanoscale.

The E-M properties of layered nanoparticles can be determined by equivalent homogeneous spheres in which the core is successively diluted into the material of the upper layers. The mixing of a dispersive material results in an equivalent Lorentzian dielectric whose properties can be fully controlled by the constitution and geometrical characteristics of the layered particle. The intrinsic resonant properties of plasmonic layered particles make them excellent candidates for nanoantenna platforms. Fig. 9 shows the complete admittance model of a nanoantenna loaded by a core-shell plasmonic particle. The particle functions as a nanoload that is used to customize the optical response of the nanoantenna by appropriately engineering its Lorentzian frequency. Note that at two frequencies the load admittance cancels the antenna’s intrinsic impedance, satisfying the antenna’s resonance condition. When the structure is illuminated by a plane wave its extinction cross-section exhibits two resonance peaks at the frequencies that the impedance model predicts. Several nanoantenna loaded structures are currently being fabricated and optically characterized.

**Deterministic Assembly:** We have initiated a new research thrust aimed at developing electric-field assisted directed self-assembly techniques to organize multicomponent nanoparticles into reconfigurable and tunable optical nanostructures, as a compelling new research direction for the renewal. In this strategy, lithographic features are designed to create a spatially varying field gradient, which is used to attract and align solutionsuspended particles at specific locations on a substrate. We investigated assemblies of metal-coated silica particles templated using dielectric posts and wells when an AC electric field is applied vertically across the solution. In the first case, the positive dielectrophoretic force attracts the highly polarizable metal particles to the regions of highest field strength at the sidewalls of the post, resulting in particle assemblies that are defined by the geometry of individual posts and post arrays (Fig. 10, top). In the second case, vertically oriented chains of nanoparticles nucleate and grow from the highest field regions at the vertices of the structures (Fig. 10, bottom). The particles can be reversibly attracted and removed as the AC field gradient is cycled. These initial results demonstrate that lithographic templates can be used to organize nanoparticles in complex arrays. Ongoing work is aimed at directed assembly of multicomponent arrays composed of particles with different optical properties.
**Future Directions:** We will continue to study hybrid optical metamaterial fabrication techniques, integrating bottom up approaches such as deterministic assembly and Au enhanced oxidation with conventional top down methods. We are developing rigorous design strategies for aperiodic, quasicrystalline geometries based on the ‘cut-and-project’ method, which models quasicrystals as lower-dimensional projections of periodic lattices in a higher-dimensional superspace.
6. Education and Human Resources

The Penn State MRSEC, the Center for Nanoscale Science, has been a leader in STEM outreach and education efforts at the University since its inception. We have a strong history of successful programs and effective collaborations, as well as a trusted position of influence and a culture that generates enthusiastic volunteers for many activities. Our size and longevity is also advantageous: we possess a breadth and depth of creative resources, and a network of connections that cross disciplinary divides and institutional boundaries. These qualities have engendered strong support from partnering entities for new MRSEC-led diversity initiatives that connect diverse participants at multiple academic levels and bridge gaps from academia to teachers, students, industry and the general public. Without the existence of the MRSEC at Penn State, many outreach and educational programs wouldn't occur at all, or would be greatly diminished in scope and scale. Many of these initiatives are led by the Center itself, while others are led by partners with direct MRSEC involvement and participation.

Center Participation: The direct personal involvement of all Center members in educational and outreach efforts is a vital ingredient for effectively integrating research into program content and an essential component for the development of well-rounded research professionals and a cohesive research community. Center faculty, students, postdoctoral scholars, researchers, and staff are expected to contribute at least 12 hours per year to outreach activities. Additionally, many former members and affiliated researchers are frequent volunteers. Several recent graduates and current students have stated that their outreach experiences were a decisive factor in employment offers and scholarship awards.

Strategy: MRSEC’s outreach and educational strategy strives to expand awareness of its research expertise, engage diverse audiences at multiple academic levels and points along the career-path, and positively impact Center members and volunteers. The Center’s interdisciplinary structure and research are areas of focus and important value-added components to the design, scope, and impact of all outreach and education efforts. Program content endeavors to communicate connections between multiple STEM fields, while emphasizing ties to current topics in materials and nanoscale science. Activities are intentionally structured to encourage interactive communication between research-oriented presenters, volunteers, and mentors with audience groups and individual participants. Target audiences include undergraduates, high school students and teachers, industry, K-12 youth, and the general public. A current Center priority is to further develop the quantity and quality of career pipelines for underrepresented and underserved groups; therefore, recruiting and retention innovations for each program are being explored,
implemented, and judged for their effectiveness. Given the Center’s large size, the logistics of engaging all members in Center activities requires a broad menu of opportunities, a simple system for participation, a low barrier of entry and commitment, and organized supportive resources.

* Programs uniquely led, organized, or hosted by the PSU MRSEC are marked with an asterisk.

**Museum Show Partnership with the Franklin Institute***

The Franklin Institute (a science museum in Philadelphia) and the MRSEC have been engaged in a longtime partnership that has resulted in the creation of five cart-based demonstration kits: *Materials Matter* (2003); *Nano-Bio: Zoom in on Life!* (2005); *Small Wonders* (2008); *Hidden Power* (2011); *Pocket Tech* (2013). The development of these kits is unique to the MRSEC at Penn State, and wouldn’t exist without the Center.

In October 2013, the 5th museum show kit, *Pocket Tech*, which explores the technology contained within personal electronic devices (such as smart phones), was awarded and distributed to 16 science museums nationwide. Recipients were small, medium, and large institutions in a variety of geographical and socio-economic areas. During 2014, this kit is expected to be seen at museums with more than 250,000 visitors. All demonstrations are designed to be hands-on, interactive, visual, and tactile. MRSEC members provided the initial inspiration and content ideas, feedback during the development process, ongoing technical oversight, and supplemental “fact sheets”. In addition, several MRSEC graduate students created prototype devices which were tested by staff at the Franklin Institute and modified to become permanent designs. AT&T provided a refurbished smart phone for each kit. Overall, 20 kits were created, with the MRSEC and Franklin Institute each retaining two copies.

*Pocket Tech* features six demonstrations that use real electronics and interactive models to explain the most notable “software” and “hardware” functions of pocket-sized computers: the binary language of data storage and processing, basic logic gates, color display technology, screen re-orientation, touch screens, and wireless signal transmission. The activities build deeper understanding of this common technology, and provide insight into emerging areas of materials science and computational research.

**Public Outreach Events**

The Penn State MRSEC continued its ongoing involvement in multiple public outreach events during the reporting period of March 1, 2013 – February 28, 2014.
Exploration-U: In early April 2013, Center members presented NISE Net demonstrations from current and previous NanoDays kits at this annual science event that exposes many young families and community members to local STEM groups and programs. Newly hosted by the Science-U outreach staff in the Eberly College of Science in partnership with the local State College Area School District, more than 600 children and adults attended the event.

Science Activities at the Central Pennsylvania Festival of the Arts – Children & Youth Day *: This annual community event each July starts with one day just for kids. Organizing and presenting science activities has been a longstanding MRSEC tradition. In recent years, these activities have expanded in both number and impact. A total of 17 booths were coordinated by the Center, 11 of which were directly staffed by MRSEC-affiliated graduate students, faculty, and staff (31 volunteers in total) who worked in teams with 41 REU students and a diverse group of 64 Upward Bound Math and Science (UBMS) high school students. The 2013 activities focused on a “Fun in the Sun” theme and included information about UV light, the nano-explanation behind clear sunscreens, solar cell technology, color and light, and how to really “cool off” with liquid nitrogen ice cream. The event is attended by ~8000 kids and adults from the local region. More than 1035 were counted as actively participating in the science activities. Given the large number of science-related booths, the overall science experience for kids makes a strong impression, and this area of the festival has become a well-known “must see” destination for many attending families.

Even deeper impact, however, was observed behind the table. While a typical child remains in front of each table for a matter of minutes, the ongoing engagement by volunteers takes place for several hours. For the second time, all teams prepared together prior to the event. Graduate students, undergrads, and high school students helped each other understand the underlying science content of each demonstration, prepare their scripts, organize tasks, and practice their presentations via role playing. Center volunteers took on leadership and mentoring roles.

Pocket Tech at Penn State “TailGreat” Event *: In October, for the third year in a row, Center volunteers engaged ~ 100 football fans before a Penn State home football game; This time, they educated the fans standing in a long line at the AT&T booth. AT&T, who donated a refurbished smart phone for each of the 20 new museum kits, eagerly supported the outreach partnership idea. The company has since borrowed the demos for its own outreach initiatives, and will feature them at the
Philadelphia Science Festival in May 2014.

**NanoDays™ at Penn State**: As a recipient of the 2013 NanoDays kit from NISE Net (Nanoscale Informal Science Education Network), the MRSEC hosted three events during April 2 – April 11, 2013. All events were organized, led, and presented by MRSEC members, but additional collaborators included the Discovery Space of Central PA, the Eberly College of Science Outreach Office, the Materials Research Institute (MRI), the Center for Nanotechnology Education and Utilization (CNEU), and Penn State’s Center for Science and the Schools (CSATS).

**Nanotechnology Workshop for Teachers**: 23 Pennsylvania K-12 educators (7 middle schools, 13 high schools; 11 males, 12 females) learned about nanoscale science and technology via a one-day workshop. Activities included a faculty presentation featuring current research, a tour of Penn State’s state-of-the-art materials characterization and fabrication facilities, the exploration of 8 NISE Net activities with graduate students and faculty, information about accessing NISE Net resources, the opportunity for high school students to remotely access and control a scanning electron microscope (SEM), a sample inquiry-based “Gecko Feet” lesson for the classroom, and information about future career opportunities in nano-related fields.

**Science Café**: The husband and wife team of Professor Matthew Thomas and Dr. Nina Jenkins from the Department of Entomology at Penn State, hosted an interactive discussion about “Bed Bugs, Small Science, Big Benefits” in a local restaurant near the Penn State campus. Their work, which focuses upon the use of fungal biopesticides for the control of malaria and has involved collaborations with materials scientists who have assisted with effectively coating netted surfaces, led to an unexpected potential solution for controlling bed bugs. MRSEC graduate students presented NISE Net activities before and after the discussion. The event was attended by 33 people (graduate students, faculty, and community members).

**“Discover the tiny World of Nano!” at Discovery Space**: MRSEC volunteers, Penn State Nanofabrication Lab staff, undergraduate engineers, and museum volunteers were prepared, using NISE Net training materials, to present kit activities at stations for a special 2-day April event at the local Discovery Space of Central PA children’s science museum. A total of 136 visitors attended.

In December, the Penn State MRSEC was again notified of its successful proposal to receive a NanoDays 2014 kit, with plans to repeat the three similar events in early April and May 2014.
Local AAUW Chapter - STEM Committee: MRSEC outreach staff continued to co-chair the STEM Committee of the local AAUW (American Association of University Women) State College Branch, while helping the committee to grow to a new total of 13 members.

- The chapter supports three afterschool science programs for middle school girls in local districts, two of which are rural – one of which was offered to girls for the first time in spring 2013.

- A “Marie Curie Science Café” public science event for adults and a “Radium Curie-osity” educational program for children were held to celebrate AAUW’s sponsorship of the element Radium in a local fundraising campaign for the local children’s museum.

- Scholarships to Science-U camps were renewed to provide deserving middle school girls with the financial opportunity to attend these enriching summer experiences.

- The new mini-grant program was renewed to support local STEM outreach efforts, and was awarded to programs such as Expanding Your Horizons (for middle school girls) and the high school workshop at the Conference for Undergraduate Women in Physics.

The involvement of MRSEC outreach staff in AAUW’s STEM efforts continued to provide the essential web of connections needed to coordinate and strengthen the partnerships formed by the recent new initiatives listed above.

K-12 Programs

Center outreach and education efforts that target K-12 audiences involve MRSEC partnerships with existing K-12 specific programs, as well as relationships with teachers, parents, school administrators, and local service organizations.

After School Science with the Center County Youth Service Bureau *: For the second year, in partnership with Penn State’s Materials Characterization Lab, the MRSEC assisted in delivering four successful interactive after school programs during spring 2013 with hands-on activities to elementary and middle school at-risk youth from the local Centre County region. Approximately 15 youth attended each program, along with their mentors or case managers. The Center will repeat the program in spring 2014 due to positive feedback from both attendees and volunteers.
**Hidden Power – Partnership with Local Elementary School Interns**: Radio Park and Ferguson Township Elementary School each welcomed MRSEC faculty and graduate students to bring *Hidden Power* museum demonstrations to the 3rd and 4th grade students as a culmination of their Energy & Electricity Unit in the spring. Approximately 80 students participated at each school, rotating through stations presented jointly by a two-person team (a Penn State elementary intern and MRSEC volunteer). This team approach was a key ingredient of the program’s success, as each presenter offered unique and important expertise to the other; interns knew how to clearly communicate with elementary kids and researchers clearly understood the scientific content within each demo. To prepare, each team worked together at a training meeting prior to the event.

**Park Forest Middle School STEM Fair**: In April, MRSEC volunteers hosted a booth, presented materials science demonstrations, and talked to students during an annual school day event that engages all 6-8th grade students and exposes them to current science topics of interest, local opportunities, and future careers in STEM fields. (~980 students enrolled)

**Park Forest Elementary School SLAM Fair**: During an evening Science, Literature, Art, and Music (SLAM) event in late April, light and optics demonstrations were presented by MRSEC volunteers to elementary families. More than 300 children and family members attended the event.

**Science-U – Science Leadership Camp**: Once again, Center volunteers contributed in multiple ways to the *Science Leadership Camp: Elements of Innovation*, a weeklong residential experience created by MRSEC for the Science-U summer camps at Penn State and attended by a diverse group of 25 high school aged youth, many of whom are recruited from outside the local community. MRSEC sponsored 13 full scholarships and assisted with the recruitment and selection of applicants from underserved and underrepresented groups.

Center faculty and graduate students hosted two groups of high school campers for a half-day, hands-on, lab-based science project in which they were given a snapshot of a particular research area or problem. One group of campers fabricated a paper microfluidic device, another learned about the unique structures, properties, and potential applications of graphene and carbon nanotubes. MRSEC faculty and graduate students also participated in the annual “scientist mixer” event, which has become a camp highlight and confirmed favorite activity.

**Summer Experience in the Eberly College of Science (SEECoS)**: During summer 2013, five MRSEC faculty members (John Asbury, Lasse Jensen, Thomas Mallouk, Theresa Mayer, and
Scott Phillips) hosted and mentored a group of diverse high school students from the Upward Bound Math and Science (UBMS) program (for low-income and first generation high school students from underrepresented and underserved populations; mentioned above regarding participation in Arts Fest). The SEECoS program provides a six-week hands-on research experience in a real laboratory setting. The SEECoS program has been in existence since the summer of 2007, and has hosted research experiences for 210 UBMS students to date. The UBMS program has an outstanding performance record: 100% of program participants graduate from high school and are accepted into postsecondary institutions; 82% graduate from postsecondary programs; 76% earn degrees in STEM disciplines.

**Higher Achievement:** In August, MRSEC continued its annual support of this program by presenting "It’s a Colorful Life: Interactions between Light and Materials" to ~80 girls and boys in the 7th-8th grades (the majority of whom are first-generation college-bound students). Participants engaged in hand-on activities to explore the absorption, reflection and refraction of light in unique materials, and learned how scientists take advantage of optical properties and behaviors to solve everyday problems.

**Haunted-U:** In October, MRSEC hosted a spooky science experience at a stop along the haunted lab tour during Science-U’s extremely popular annual Halloween-themed science program. During the half-day event, 80 upper elementary and middle school students learned about “viral outbreaks” before being joined by ~100 parents for the evening tour.

**Ferguson Elementary Science Expo:** In February 2014, MRSEC graduate students, a research associate, and an outreach staff member brought *Pocket Tech* to the public for the first time at a local elementary school science fair. More than 50 students, plus siblings and parents, attended. One parent, an elementary school teacher in a much more rural district in Central PA, inquired about bringing the demonstrations to their school in May 2014.

**Expanding Your Horizons (EYH):** Also in February, MRSEC facilitated a panel discussion that engaged more than 100 middle school aged girls and their parents, along with more than 30 graduate and undergraduate mentors. The panel included faculty, graduate students, and undergrads who answered questions about the pursuit of STEM degrees and careers. The event, hosted by Eberly College of Science outreach staff, also included a science expo, and three interactive workshops.
Research Experiences for Undergraduates and Teachers

*Research Experiences for Undergraduates (REU):* In partnership with the Department of Physics, the Center is designated as a REU site by the National Science Foundation Division of Materials Research (DMR 1062691). Undergraduate students majoring in physics, chemistry, materials science, and all branches of engineering who have an interest in materials research are encouraged to apply. This program provides undergraduates with the opportunity to participate in frontier materials and physics research with broad exposure to unique interdisciplinary projects and cutting-edge facilities.

Required attendance at weekly seminars ensured that students were informed about the broad scope of interdisciplinary research, career opportunities and educational strategies, and ethics issues. Additionally, valuable professional development experiences occurred via an educational trip to the Franklin Institute science museum (where students learned about the design and development of museum exhibits, and the importance of informal science education programs), participation in the Central Pennsylvania Festival of the Arts Children and Youth Day (described above), and the large joint Summer Research Symposium structured to simulate the feel of a professional conference (where students presented their summer research via a poster session and 10-minute talk).

In the summer of 2013, the MRSEC also initiated and implemented a new joint REU program series as part of its strategic plan to increase the representation and success of underrepresented and underserved individuals in STEM fields. While each REU program at Penn State is distinct in its research focus, there exists both a need and value-added opportunity to coordinate some initiatives across all programs. The primary goal of the series, titled “Different Science, Different People, Working Together”, is to create a welcoming campus climate and larger, supportive summer research community where participants are exposed to an even broader array of potential future research opportunities. A successful proposal to the Equal Opportunity Planning Committee at Penn State resulted in an initial grant award, as well as an invitation to resubmit for continued funding in summer 2014. The three part series, included a Welcome Orientation with a diversity training workshop, a special seminar series featuring broad-stroke topics such as “communicating science to the public” and a tour of Penn State’s new materials characterization and fabrication facilities, and a networking and team-building event which focused upon the interdisciplinary nature of current research. (Additional information is provided in section 8.)
The MRSEC directly supported the following 4 undergraduates during the summer of 2014:

<table>
<thead>
<tr>
<th>Student</th>
<th>College or University</th>
<th>Faculty Mentor</th>
<th>Research Project Title</th>
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</thead>
<tbody>
<tr>
<td>Matthew Bauer</td>
<td>Clarion College</td>
<td>Theresa Mayer</td>
<td>Minimization of Order Disruptions in the Drying Process of Dielectrophoretically Assembled Nanoparticles through Lyophilization and Cooled Evaporation</td>
</tr>
<tr>
<td>Kathleen Maleski</td>
<td>Washington College</td>
<td>Vincent Crespi</td>
<td>How to put a tetrahedron into a plane: sp3 defects in sp2 carbon</td>
</tr>
<tr>
<td>Christopher Rotella</td>
<td>Rowan College</td>
<td>Mauricio Terrones</td>
<td>Carbon nanotube networks</td>
</tr>
<tr>
<td>Victor Vivas Lopez</td>
<td>University of Puerto Rico, Cayey</td>
<td>Thomas Mallouk</td>
<td>Transforming non-polar Ruddlesden-Popper layered perovskites to produce ferrielectrics</td>
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</tbody>
</table>

The following 13 MRSEC faculty mentors hosted 16 undergraduates in their laboratories to complete projects related to MRSEC research activities:

(Note: This list includes the MRSEC funded students above.)

<table>
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<tr>
<td>John Badding</td>
<td>Daniel Long</td>
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<td>High Pressure Chemical Vapor Deposition Fluid Flow in Microscale Capillaries</td>
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<td>Vincent Crespi</td>
<td>Kathleen Maleski</td>
<td>Washington College</td>
<td>How to put a tetrahedron into a plane: sp3 defects in sp2 carbon</td>
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<td>Enrique Gomez</td>
<td>Larry Morton</td>
<td>University of Maryland, Baltimore County</td>
<td>Optical and Structural Characterization of Conjugated Block Copolymers</td>
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<tr>
<td>Tony Huang</td>
<td>Justin Kiehne</td>
<td>Dickinson College</td>
<td>Portable Molecular Diagnosis Using Surface Acoustic Waves</td>
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<tr>
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<tr>
<td>Susan McKinstry</td>
<td>Michael Vecchio</td>
<td>Dickinson College</td>
<td>Prototype SMART-X Mirror Panel Fabrication for Lifetime Testing</td>
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<tr>
<td>Joan Redwing</td>
<td>Nerrissa Mitchell</td>
<td>University of New Orleans</td>
<td>Annealing and Characterization of Bismuth Selenide Thin Films</td>
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<tr>
<td>Name</td>
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<td>Institution</td>
<td>Project Title</td>
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<td>Ausyman Sen</td>
<td>Antonio Ramos</td>
<td>University of Puerto Rico, Cayey</td>
<td>Hierarchical assembly and sorting of active and inactive particles</td>
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<td>Jorge Sofo</td>
<td>Michael O'Boyle</td>
<td>State University of New York, Geneseo</td>
<td>Hydrogen Bonding on the SiO2 (101) Surface and Its Relation to Dissolution</td>
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<td>Synthesis of Phosphorous-doped Graphene and its enhanced Raman scattering effect</td>
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<tr>
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<td>Raman Spectroscopy studies of few layered WSe2</td>
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<td>Darrell Velegol</td>
<td>Humberto Gonzalez-Ribot</td>
<td>University of Puerto Rico, Mayaguez</td>
<td>Designing hierarchical micro-structures inside capillaries through diffusioosmotic flows</td>
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<tr>
<td>Jun Zhu</td>
<td>Tyler Haussener</td>
<td>Susquehana University</td>
<td>Negative Difference Resistance in Monolayer Graphene p-n Junctions</td>
</tr>
</tbody>
</table>

In addition to the Physics/MRSEC REU program described above, MRSEC faculty were also actively involved in several other summer research experience programs for undergraduates:

- Five current faculty members (John Asbury, John Badding, Lasse Jensen, Scott Phillips, and Raymond Schaak) were advisors for participants in the REU and 3M programs hosted by the Department of Chemistry, College of Science.
- Two faculty members (Enrique Gomez and Darrell Velegol) supervised a student in the REU program in Soft Materials hosted by the Materials Science and Engineering Department, College of Earth and Mineral Sciences.

The strong involvement by PSU MRSEC faculty in multiple REU programs (each with a specific and unique research focus) demonstrates the extent to which the Center is, directly and indirectly, exposing and promoting interdisciplinary research to the next generation of researchers.

Note: The statistics reported for the Physics/MRSEC REU program in Appendix C (Number of Active Participants) include additional students from other funding sources. At no additional expense, the program strives to broaden the impact of its NSF funding by including all physics-affiliated summer research students in the career development activities organized for the REU students. Those receiving direct MRSEC financial support are specifically shown in the right-hand column. Without the existence of the MRSEC, the majority of joint activities and several professional development experiences would not take place.
First Year Research Experiences for Millennium Scholars: The brand new Millennium Scholars undergraduate program, initiated by Penn State’s Eberly College of Science and College of Engineering, welcomed its first class of 19 diverse scholars during the summer of 2013, all of whom have committed to the future completion of a PhD. Research experiences are required annually by the program, starting no later than the scholar’s very first summer (2014). All scholars are also required to complete an undergraduate research thesis, and are encouraged to secure a faculty research advisor during their first year. Given the importance of making this early connection with a Penn State faculty member, as well as the known competitiveness of REU programs at other universities (i.e. the unlikely acceptance of first year students), the MRSEC provides summer support for five first year scholars who are matched with MRSEC faculty and projects. As a result, strategic matching efforts were implemented during the fall and winter to assist both scholars and MRSEC faculty in identifying a shared research interest and making a viable connection.

Interdisciplinary Research Experience for Teachers Program (RET): In partnership with the Department of Physics, which has been designated a RET site by the National Science Foundation Division of Materials Research (DMR 1062691), and MRI’s NanoFab facility, the MRSEC provided multiple avenues of support for the program. Francelys Medina, a MRSEC postdoctoral fellow, coordinated all aspects of the application and recruitment of teachers, matched faculty advisors and projects with teachers, organized technical and educational seminars and workshops, confirmed and supported the participation of the teachers in the Symposium, implemented evaluations, and provided ongoing logistical and personal oversight as needed. Participants received 3.5 graduate credits from Penn State, as well as 30 hours of Pennsylvania Act 48 credit. Additional MRSEC support included faculty advisor participation, funding for project materials, staff support for preparing presentations at the Summer Research Symposium.

The goal of the six-week RET program at Penn State is to provide opportunities to the participating STEM teachers to engage in hands-on research projects with faculty mentors in materials and nanotechnology. Teachers who are better prepared in science content and who themselves have developed hands-on activities will contribute to enhancing the quality of STEM instruction. Teachers worked together in the development of lesson plans, oral and poster presentations, and papers for publication. MRSEC researchers are building collaborative relationships between K-12 teachers and the research community, supporting the active participation of in-service teachers and pre-teachers in research and education projects, and
providing the students of the RET participants with the appropriate content, skills, and career information to influence their future careers and competition in STEM education. In addition, after completing the summer program, teachers are encouraged to apply for a mini-grant to implement research-related science experiments in their classrooms.

The following six teachers participated in the 2013 RET program, all hosted by current and/or affiliated Center faculty:

<table>
<thead>
<tr>
<th>Teacher</th>
<th>School</th>
<th>Faculty Mentor</th>
<th>Research Project Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>Terri L. Ogden</td>
<td>Philipsburg-Osceola</td>
<td>Christine Keating</td>
<td>Evaluating the Effects of Surfactants on Surface Tension Evaluating the Effects of in the High School Classroom</td>
</tr>
<tr>
<td>Cortney C. Wright</td>
<td>Bedford County Career &amp; Technology Center</td>
<td>Christine Keating</td>
<td>Evaluating the Effects of Surfactants on Surface Tension Evaluating the Effects of in the High School Classroom</td>
</tr>
<tr>
<td>Joyce Theriot</td>
<td>Rustin</td>
<td>Roman Engel-Herbert Nasim Alem</td>
<td>Zooming into the Atomic Arrangement of Nanostructured Crystals</td>
</tr>
<tr>
<td>Adria M. Bondanza</td>
<td>Sun Valley High School</td>
<td>Roman Engel-Herbert Nasim Alem</td>
<td>Zooming into the Atomic Arrangement of Nanostructured Crystals</td>
</tr>
<tr>
<td>Steven K. Schulz</td>
<td>Manheim Township</td>
<td>Ayusman Sen</td>
<td>Glucose Effects on the Schooling or Exclusion Behavior of Silver Phosphate Microparticles Under Different pH Conditions</td>
</tr>
<tr>
<td>Craig A. Fink</td>
<td>Philipsburg Osceola</td>
<td>Thomas Mallouk</td>
<td>Characterizing Emergent Properties of Magnetic Nanowire Motors</td>
</tr>
</tbody>
</table>

**Recruitment and Retention**

*Fall STEM Preview Open House*: In September 2013, Penn State held its first STEM Open House for prospective graduate students, hosting more than 30 underrepresented and underserved minority and female undergraduate students in their junior or senior year. The idea for this event came from the MRSEC diversity committee and MRSEC personnel spearheaded the first run of the program. Led by former MRSEC outreach faculty member, Dr. Ron Redwing, the MRSEC committed to providing inaugural financial support, program leadership, and staff support. Center faculty also served as speakers, panelists, and departmental hosts. Due to the MRSEC’s impetus, committed involvement soon followed by the MRSEC’s three affiliated colleges and The Graduate School. Such a preview event, before the graduate application process is in full swing appears to be a common best-practice by universities and colleges who have strong and successful track records of attracting and
retaining diverse student populations at the graduate level. Positive feedback from attendees after the event resulted in expanded participation interest by other colleges for fall 2014, and permanent central planning leadership by The Graduate School. The Graduate School will also evaluate the program and track the final graduate school decision made by attendees. The MRSEC will continue to play a central role in the program as a primary partner on the planning committee, and strong participation by Center faculty in the program itself, and departmental activities.

Conference for Undergraduate Women in Physics (CUWiP): Penn State was provided with the opportunity to host the 2014 Northeast Conference for Undergraduate Women in Physics, held in January. Organized by the Physics and Astronomy for Women (PAW) group, MRSEC provided financial support, recruitment efforts by faculty during the Graduate School & Career Information Fair, and a workshop presentation by outreach staff on the topic of “Effective Networking”. In addition, the MRSEC outreach staff was utilized frequently as a resource by the planning committee. More than 140 female undergraduates registered to attend, and the successful results of the planning committee earned PAW members an invitation to share their experience at the APS March Meeting.

Women in STEM Mixer *: In partnership with PAW, the MRSEC spent several months planning the Women in STEM Mixer, scheduled to be held at the end of March 2014. The chosen theme “Mentors and Mentees – Creating a Win-Win Relationship” will be discussed by 80 participants (20 undergraduates, 30 graduate students, 10 researchers or staff, 10 research faculty Hosts, and 10 industrial partner Co-hosts) in a three-part networking format which intentionally brings multiple career levels together. Additionally, making connections with industry partners and obtaining their viewpoint in the discussions is viewed by attendees as another important strength of the program. The event also provides non-local industry Co-hosts with the impetus to arrange in-person meetings with current faculty partners and others who may be interested in future collaborations.

Evaluation & Assessment

Evaluation and assessment efforts of education and outreach initiatives are designed separately for each program, depending upon particular goals and desired outcomes, and implemented accordingly. In addition, keeping accurate and detailed records of all education outreach efforts and volunteer contributions remains a priority of the Center. The collected information is used to assess the beneficial impacts on both volunteer presenters and participants, acknowledge and recognize the contributions made by MRSEC members, and identify needed program changes and improvements.
MRSEC Education Director Network - Evaluation Committee: Kristin Dreyer continues to serve as Co-chair of the Evaluation Committee for the MRSEC Education Directors Network. The following was discussed during the September 2013 meeting:

Charge Statement: Facilitate multi-center usage of common evaluation instruments† to (1) collaboratively assess MRSEC value-added impact of similar education programs and goals, (2) determine best practices, and (3) communicate findings to NSF* and the MRSEC Education Network.

† Note: Common usage may entail either whole or partial instruments.

* Rationale: Multi-center evaluation is needed by NSF MRSEC leaders to advocate funding to Congress for the MRSEC program.

Committee Goals for 2012-13: Establish broad multi-center participation and joint follow-up analysis using existing common evaluation tools for recent (2010-2012) and upcoming REU (2013) and RET programs and identify additional commonalities that may exist among MRSEC Centers.

Outcomes of the meeting were mixed. Existing evaluation tools were reviewed for REU and RET programs, but no usable tools (or partial tools) emerged as intended. Therefore, subsequent multi-center participation was not sought. Instead, the committee started focusing upon the value-added impact of Center activities upon Center research members themselves. Impacts due to participation in MRSEC-specific activities during membership, as well as long-term tracking of member career paths, were areas of focus that may generate meaningful metrics and a sharable multi-site system of data collection and comparison. More work on this focus area is intended prior to and during the 2014 meeting.

REU and RET Programs: Both the REU and RET programs associated with the MRSEC use multiple evaluation measures. The REU program conducted an initial background survey, two formative surveys to assess the program experience while in progress, and a final summative post-survey. The data collected was utilized internally by program coordinators. The RET program once again participated in the multi-site evaluation program conducted through Columbia University. Penn State compared favorably to other schools. Penn State specific results indicated that all but one teacher felt that their experience will have an impact on student achievement in their classes, and that the experience increased their interest in research and the ways that science can be applied.

In 2013, the brand new MRSEC lead “Different Science, Different People, Working Together” joint program activities were assessed in multiple ways to indicate the extent of their
effectiveness. For example, the attendees at the diversity training workshop demonstrated a 75% average increase in their understanding of diversity, measured by pre-post tool (79 students attended); at the networking mixer, records submitted on paper slips indicated that the 75 attendees made 146 interdisciplinary connections with other researchers; and metrics collected at the final poster session indicated that each poster was meaningfully visited by more than 3 fellow researchers in one hour, many of whom were from other REU programs. A detailed report was submitted to the University’s Equal Opportunity Planning Committee (EOPC) as a follow-up requirement for their financial support. EOPC later contacted the MRSEC to invite a resubmission of the proposal for summer 2014, and subsequently awarded funding to it for the second time.

Hands-on museum kits activities are also continuously assessed, through short post-interaction surveys administered to museum visitors during kit development, to guide both adjustments to demo hardware and to the scripting and background information for presenters.
7. Postdoctoral Mentoring Plan

The MRSEC hosts postdoctoral researchers in two distinct types of positions: research-focused postdoctoral fellows and also education/outreach postdoctoral officers. These two positions have a distinct character, but share many common mentoring goals. We begin by describing the elements in common to both types, and then describe the elements that are unique to each.

Each postdoctoral fellow, working in conjunction with appropriate lead faculty members (faculty research mentors or the Associate Director in charge of outreach), is expected to develop an Individual Development Plan (IDP). The IDP outlines long-term career goals and short-term objectives, identifies areas for specialized training, and facilitates effective communication of expectations between postdoc and mentors. The mentors provide the postdoctoral fellow with counseling tailored to his/her career goals in academia, industry or government. These plans are based on published best practices as presented in the National Postdoctoral Society mentoring toolkit. Depending on their interests and goals, the postdoctoral scholar is offered training opportunities ranging from research training to formal workshops, seminars, informal mentoring, opportunities to supervise more junior researchers, research presentations. Key components of a mentoring plan include:

- Introduction to the local environment and campus-wide resources available to support their research, teaching, outreach and professional development.

- Participation in the Scholarship and Research Integrity program at Penn State to provide comprehensive training in the responsible conduct of research.

- Participating in a brown-bag lunch series (sponsored by the Penn State Postdoctoral Society) where speakers discuss leadership, professional ethics, work-life balance, conflict resolution, career paths in and outside of academia, entrepreneurship, applying for positions and negotiating start-up packages.

- Presentations in MRSEC seminars to develop communication and presentation skills.

- Guidance with regards to a journal club organized by the Penn State Graduate School to provide guidance on writing scholarly publications.

- Travel to at least one professional conference each year to present the results of research, develop professional relationships and network with colleagues.

- Networking with leaders in academia and industry by meeting with them during campus visits and at professional meetings.

- Attending seminars and workshops on how to identify funding opportunities and write competitive grant proposals that are offered by the Office of Postdoctoral Studies. Involvement in MRSEC-oriented proposal preparations at the Seed level and also related proposals (PREM, REU, etc.)

- Participating in seminars on improving teaching effectiveness offered by the Schreyer Institute for Teaching Excellence. Examples include “Understanding and Engaging Today’s University Student” and “The Future of Textbooks in the Digital Age.” Postdoctoral scholars who intend to pursue academic positions are encouraged to teach at least one undergraduate course in their academic discipline during their time in the Center, and to obtain formal eval-
ations from their students. This is a particular focus for the postdoctoral education/outreach officers (as described below) but the opportunity is available to all.

In addition, research-focussed postdoctoral fellows participate in regular IRG-level and smaller-scale research meetings to present and discuss results, brainstorm future directions, and plan publications. Research postdocs are intended to act as “glue” within an IRG, interacting across individual research groups and thereby obtaining broad, interdisciplinary perspective and capabilities. Through the sharing of problem solving strategies, the postdoctoral researchers gain experience in making sensible short and long term decisions to get the most out of a research project. Since all post-docs come with different skill set, strengths and weaknesses, career plan and personality, it is necessary to tailor a mentoring plan to best fit each individual, with particular focus on communication skills, specific research expertise, academic versus industrial versus teaching goals, etc. The MRSEC has had good success in the next stages in postdocs’ career paths; for example, out of a set of 21 recent postdocs across a wide range of research topics, twelve obtained faculty positions, eight are currently working as research scientists or administrators in universities, national laboratories and private industry, one is teaching high school and one is a post-doc in a national lab.

Education/outreach postdoctoral fellows typically have a distinct set of career goals, and our mentoring plan reflects these so that each postdoc can develop a compelling, balanced portfolio of experiences and accomplishments that cover the range of capabilities – teaching, grant writing, outreach, and research. To ensure that adequate mentoring is provided in in teaching, we target co-teaching environments, either as one lecture section in a multi-track introductory course or as one of two instructors co-teaching an upper-level undergraduate course. Further mentoring is provided in the joint preparation of grant proposals: one prior outreach postdoc successfully obtained an NSF Discovery Corp fellowship; another led the effort to prepare and submit a successful REU site proposal. Future opportunities along these lines may include the PREM, I-Corps, REU (renewal) programs and other venues. We also provide opportunities for education/outreach postdocs to maintain a research arm to their activities, hosted in a MRSEC lab. In this manner, they can build a compelling CV that demonstrates success in teaching, securing grant resources, publishing, and a portfolio of outreach efforts that span from museum/academia partnerships to designing curricula for summer camps, working with high school teachers, etc. In addition, all postdocs are encouraged and supported to attend disciplinary and professional development conferences and workshops. As a measure of success, four recent education/outreach postdocs have all secured permanent teaching positions, and our prior instructor-level education/outreach manager is now an associate dean. This mentoring is the primary responsibility of the Associate Director for Outreach, but other faculty participate as well as appropriate.

This mentoring program is assessed by regular discussion and feedback on each IDP as well as by the success in achieving career goals both during and following the postdoctoral fellowship. The Center Director consults on an annual basis with the primary faculty mentors of each postdoc to monitor career progress and ensure that each postdoctoral fellow has a comprehensively supportive environment for career development.
8. Center Diversity – Progress and Plans

*Diversity Strategy Overview:* The Penn State MRSEC has recognized that, in order to further increase the diversity of our own Center participation, we need to target institutional-level change. We are addressing pipeline issues of recruiting, support and retention by nucleating institutional-level efforts. While continuing the historically most effective diversity-focused efforts that have provided *consistent representation of female and URM participants that exceeds departmental levels*, three brand new initiatives were fully implemented during the past year. The foundation of two additional strategic programs has also been laid in preparation for immediate implementation at the start of our successful renewal. Increasing Center participation of women and diverse individuals, institutions, and geographical areas requires a strategy that acknowledges the importance of *reaching multiple positions along the career pathway* and the connections between these positions. There are inherent challenges associated with the fact that actual graduate student involvement in Center research activities usually begins long after admission to a doctoral program. Therefore, the strategy incorporates *short-term activities, aimed at broadening immediate participation*, as well as growing the number of *long-term partnerships to help open and build more channels of entry*. To do so, recent initiatives have emphasized *broader engagement of Center faculty*, expanding their involvement and investment in this initiative, discovering new connections through their professional contacts, and increasing their overall awareness of the goals. Further, in order to both attract and retain diverse students at Penn State, the Center is striving to diversify Center faculty membership.

*Center Participation:* In previous years, we separated our membership data into three categories: Faculty, Postdoctoral Fellows, and Graduate Students. In addition, to obtain meaningful metrics for assessing institutional level change, we compared Center percentages in these categories to those of our constituent departments in 2012 to establish a benchmark against which to track longitudinal data. However, as per the guidelines outlined for this reporting period, Center data are now collected directly by NSF, and do not contain such categorical distinctions. As a result, the three categories have been compressed for 2013 data. Further, departmental comparisons are not meaningful and are therefore not included in this report.

<table>
<thead>
<tr>
<th>2013 Total</th>
<th>Women in MRSEC</th>
<th>Underrepresented Minorities (URM) in MRSEC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Faculty, Postdocs, Graduate Students*</td>
<td>83 respondents (out of 110)</td>
<td>23/83 (28%)</td>
</tr>
<tr>
<td>REU (Undergraduates)</td>
<td>18</td>
<td>6 (33%)</td>
</tr>
<tr>
<td>RET</td>
<td>6</td>
<td>4</td>
</tr>
</tbody>
</table>

Table 1: Summary of 2013 participants by category of Women and Underrepresented Minorities (URM)
The consistency of the longitudinal numbers below, when considered relative to total participation, indicates the Center's ongoing commitment to diversity, but also demonstrates that there exists a limitation at the institutional level that is preventing further progress. As a result, the Penn State MRSEC is now taking an active leadership position in broadening the participation of its constituent departments – with the ultimate goal of increasing the diversity of both the Center and the departments - through several new, strategic initiatives.

<table>
<thead>
<tr>
<th>Year</th>
<th>Faculty</th>
<th>Post</th>
<th>Grad</th>
<th>REU</th>
</tr>
</thead>
<tbody>
<tr>
<td>2003</td>
<td>48</td>
<td>7</td>
<td>34</td>
<td>26</td>
</tr>
<tr>
<td>2004</td>
<td>49</td>
<td>10</td>
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</tr>
<tr>
<td>2005</td>
<td>50</td>
<td>11</td>
<td>36</td>
<td>32</td>
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<tr>
<td>2006</td>
<td>42</td>
<td>11</td>
<td>40</td>
<td>32</td>
</tr>
<tr>
<td>2007</td>
<td>38</td>
<td>13</td>
<td>38</td>
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<tr>
<td>2008</td>
<td>45</td>
<td>19</td>
<td>57</td>
<td>21</td>
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<tr>
<td>2009</td>
<td>43</td>
<td>12</td>
<td>46</td>
<td>20</td>
</tr>
<tr>
<td>2010</td>
<td>49</td>
<td>12</td>
<td>56</td>
<td>18</td>
</tr>
<tr>
<td>2011</td>
<td>45</td>
<td>9</td>
<td>52</td>
<td>13</td>
</tr>
<tr>
<td>2012</td>
<td>49</td>
<td>10</td>
<td>62</td>
<td>19</td>
</tr>
<tr>
<td>2013</td>
<td>43</td>
<td>11</td>
<td>56</td>
<td>18</td>
</tr>
</tbody>
</table>

Table 2: Total Number of Penn State MRSEC participants by year and category

<table>
<thead>
<tr>
<th>Year</th>
<th>Faculty</th>
<th>Post</th>
<th>Grad</th>
<th>REU</th>
</tr>
</thead>
<tbody>
<tr>
<td>2003</td>
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<tr>
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</table>

Table 3: Number of Penn State MRSEC Women participants by year and category

<table>
<thead>
<tr>
<th>Year</th>
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<th>Post</th>
<th>Grad</th>
<th>REU</th>
</tr>
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<tr>
<td>2013</td>
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<td>3</td>
<td>4</td>
<td>8</td>
</tr>
</tbody>
</table>

Table 4: Number of Penn State MRSEC Underrepresented Minority participants by year and category

**New Connections with URM Undergraduate Programs:** The MRSEC has been part of a new program, initiated by the Eberly College of Science at Penn State and developed in consultation with the leaders of the *Meyerhoff Scholars program at the University of Maryland, Baltimore County (UMBC).* Meyerhoff is an undergraduate program that has successfully supported underrepresented minority students in their pursuit and achievement of doctoral degrees in science, engineering and mathematics. Penn State is using UMBC’s program as a model for its *Millennium Scholars* initiative, which launched in summer 2013. The ideas shared by Meyerhoff during the planning process in 2012 focused on the key components of their success, and articulated many **best practices.** The Center requested to participate in these activities, as well as meet personally with program leaders. These best practices were summarized by Keith

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* Source: NSF survey results; data does not distinguish between Faculty, Postdoc, and Graduate Student; 83 out of 110 Center participants responded to the survey (110 = 43+11+56; see table below)
Harmon, Director, when he said, “At the end of the day, it’s all about building relationships”, because positive relationships build the solid community foundation that attracts and retains minority and underserved individuals. As a result, the Center realized that permanent, positive increases in diverse participation numbers requires a multi-sided, personalized, long-term approach to diversity-oriented education, recruitment, and retention activities that foster interpersonal communications, an inclusive and supportive atmosphere, and a vibrant sense of community. Such a goal can’t be achieved by the isolated efforts of a few key people; therefore, the MRSEC implemented new recruitment and retention activities in 2013 that include involvement at all levels of Center membership.

**Research Experiences for Undergraduates (REU):** Summer research participation throughout the entire four year period is a requirement of all Meyerhoff and Millennium scholars. As a result, a continued effort was made in 2013 to recruit REU applicants from the Meyerhoff program via direct communication with Meyerhoff directors, as well as a campus visit and presentation by Dr. Jorge Sofo, principal investigator of the Physics/MRSEC REU program ((DMR 1062691), in November 2013. More than 40 Meyerhoff scholars attended the talk, all majoring in the physical sciences, and six requested individual meetings following the presentation.

Given the highly competitive nature of the REU program, and the advanced level of many of the current project areas proposed by participating Penn State faculty mentors, successful REU candidates tend to be rising juniors and seniors. However, the need for first year research experience opportunities has been identified, as well as the unique support structures and program elements that are necessary in order to provide meaningful and positive experiences to younger undergraduate scholars. As a result, **MRSEC faculty members were matched with five Millennium Scholars to conduct summer research in 2014**, and these first year students will be supported by the Center. These faculty members will likely become thesis advisors for these students, and continue to work with them throughout the next three academic years.

The Center, through continued efforts by Dr. Ronald Redwing, also maintained its traditional presence at national scientific conferences hosted by organizations dedicated to the advancement of underrepresented minorities in STEM. Dr. Redwing, now the Associate Dean for Educational Equity in the College of Earth & Mineral Sciences, is a longtime MRSEC faculty member who formerly managed many of MRSEC’s education, outreach, and diversity initiatives. He continues to support the Center in his current role. Through his participation at national conferences, school visits with faculty and students, networking with attendees, and presentations, undergraduates were informed about MRSEC-affiliated summer research programs and opportunities for future graduate studies.

A new, joint **REU program series, titled “Different Science, Different People, Working Together”** was successfully implemented during summer 2013. Participation included all MRSEC-affiliated REU programs, as well as other summer undergraduate research students. This joint series included three parts, the first being a welcome orientation with diversity
education and community-building activities. It provided a clear message regarding the value of diversity in science and engineering, as well as the growing trend of interdisciplinary research. A seminar series, titled *The Millennium Mash-up*, was held at the new Millennium Science Complex building, home of several state-of-the-art user facilities and laboratories, as well as Penn State’s Materials Research Institute (MRI) and the Huck Institute for the Life Sciences. Finally, a professional networking and team-building event provided another opportunity for students to become engaged with the larger research community, and exposed to the tremendous variety of people, facilities, and research that Penn State has to offer. (See Section 6 for further details.) Evaluation efforts successfully measured an increase in participants understanding of diversity, and provided strong evidence that the activities promoted a welcoming and inclusive community environment. The program received endorsement at many levels. Penn State’s Equal Opportunity Planning Committee (EOPC), under the direction of the Office of the Vice Provost for Educational Equity, awarded the initial grant to support this REU program series, and invited the Center to submit for continued funding in summer 2014 (which was also awarded).

**Graduate Recruitment, Admission, and Appointment Processes:** The MRSEC Diversity Committee has become engaged in consistent, purpose-driven communications with many stakeholders: the Center faculty, affiliated department graduate admissions committees, college-level multicultural officers, and Penn State’s Graduate School. The primary recent focus of the committee has been to identify new opportunities for unique, value-added participation and support by the PSU MRSEC in graduate student recruitment efforts to attract and attain a greater number of top-level underrepresented, underserved, and female graduate students. *A larger initial pool of diverse incoming students is needed in order to realize greater increases in MRSEC membership over the months and years ahead.*

As a result, several new institutional-level initiatives are underway. First, *greater direct involvement by Center members in diversity recruitment and retention activities* has been designated as a specific new outreach category in which they can contribute their time and personal enthusiasm. Such activities will involve representation of the MRSEC at department and college level graduate recruitment events, hosting tours and information sessions, serving on graduate admissions committees of MRSEC-affiliated departments, representing the Center at national conferences and events, etc. This community-minded approach strives to establish relationships with new students, make the PSU MRSEC a more visible and tangible entity to incoming graduate students at the very start of their Penn State career, and provides the opportunity for current members to become more fully aware of the breadth and depth of the Center’s research activities. Greater involvement of current MRSEC faculty in the processes that occur in their respective departments (from the period of recruitment and admission to the time of graduate appointments), with mindfulness regarding the importance of a diverse MRSEC membership, is intended to improve the probability that student pathways may ultimately lead to MRSEC projects. These new activities are being implemented in the current recruiting cycle. Therefore, results will not be realized until next year, and evaluation of the long-term impact of these initiatives will take several years. However, these initiatives closely follow the best practices articulated by Meyerhoff leaders as key elements of success.
During an icebreaker activity, faculty members engage in conversations with STEM Open House attendees about the many applications of nanotechnology.

One particularly exciting, new University-wide program – a Fall Preview STEM Open House (conceived by the MRSEC Diversity Committee) was held for the first time in September 2013, attended by 31 underrepresented and underserved minority undergraduate and female students in their junior or senior year. Such a preview, before the graduate application process is in full swing, appears to be a common best-practice by universities and colleges who have strong and successful track records for attracting and retaining diverse student populations at the graduate level. MRSEC committed the initial financial support, prompting the partnering Colleges to follow. Dr. Ronald Redwing took the lead on organizing the event, together with several members of the MRSEC Diversity Committee and MRSEC staff. MRSEC faculty hosted students for departmental tours, attended networking sessions and dinners, gave presentations, and served as panelists.

In an effort to have a greater influence on diversity in graduate recruiting, the MRSEC-MRI Fellowship program was re-structured. In the past, the Fellows were senior MRSEC students with a strong track record of research accomplishments. The program will now more broadly solicit nominations of incoming first-year graduate students who demonstrate an interest in joining one of the IRGs or seed projects.

Supporting Women and Girls in STEM: The Center implemented several new efforts to support the success of female students and researchers at Penn State, targeting multiple positions along the career-path. In addition, the rural geographical location of the Penn State community within Central Pennsylvania gives the MRSEC a unique opportunity to impact a local female population that is lacking opportunities, encouragement, and support to pursue success in STEM fields. As a result, the Center has been strategically seeking, developing, and becoming involved in new initiatives, programs, and partnerships that target, in particular, the young women and girls within nearby communities.

The Center’s unique umbrella position, tradition of successful outreach endeavors, and many strong partnerships within the University community helped to reinvigorate the STEM Committee of the local State College Branch of the American Association of University Women (AAUW). Continuing to serve as Co-chair of the committee, Kristin Dreyer, MRSEC Program Director of Education and Outreach, worked to expand the committee (~13 people now serve) and implement the multiple new initiatives started the previous year. (Details can be found in Section 6.)

Penn State was chosen to host the 2014 Northeast Conference for Undergraduate Women in Physics (CUWiP) in January. Organized by the Physics and Astronomy for Women (PAW) group, MRSEC provided financial support, recruitment efforts by faculty during the Graduate School & Career Information Fair, and a workshop presentation by outreach staff on the topic of “Effective Networking”. In addition, the MRSEC outreach staff was utilized frequently as a resource by the planning committee. More than 140 female undergraduates registered to attend, and the successful results of the planning committee earned PAW members an invitation to share their experience at the APS March Meeting.
The Center is hosting its 2nd *Women in STEM Mixer* on March 2014, in partnership with the Physics and Astronomy for Women (PAW) student organization. This retention-oriented multi-level professional networking event will focus on “the mentor/mentee relationship” and feature presentations and participation by academic research faculty hosts and industry representative co-hosts. For the second time, the tremendous response to minimal marketing efforts demonstrates both the appeal and need for such an event. (See Section 6 for additional details.)

**Incorporating Diversity into K-12 Initiatives:** MRSEC provided scholarships to 13 diverse high school campers (6 female, 11 URM) for a unique weeklong residential experience at *Penn State’s Science Leadership Camp*, which is part of the *Science-U* summer camp program. Changes made by the MRSEC to the scholarship marketing and application process successfully resulted in a larger pool of competitive applicants who were more geographically and ethnically diverse. Evidence of financial need was a baseline criterion, while enthusiasm for science, the desire to develop leadership qualities, and personal character traits were highly considered for final selections.

The *Summer Experience in the Eberly College of Science (SEECoS) research project* is a 6-week program in which small groups of 3-4 high school students from disadvantaged schools each conduct a simple, structured, research-like project with the assistance of undergraduate, graduate, and faculty mentors in a real laboratory. Five MRSEC faculty members hosted groups. The students are part of the tremendously successful Upward Bound Math and Science (UBMS) program (which, in 2013, served 70 low-income and first generation students from underrepresented and underserved populations). These UBMS students were also placed in teams with Physics/MRSEC REU students, MRSEC faculty, and MRSEC graduate students to participate in a full day of science outreach during the local Arts Festival Kids Day event.

**Long-term Communication Benefits:** The history of the Meyerhoff Scholars program at UMBC has demonstrated that the impact of summer research experiences is by far not limited to the individual participants themselves. After completing the program, the participant’s entire personal network of friends and classmates receive information about the perceived quality of that student’s experience and his/her future opportunities. Therefore, whether positive or negative, there is tremendous potential for ripple effects to occur. When wisely realized, these effects can be constructively capitalized. Such knowledge also lends rationale to the importance, potential benefits, and effectiveness of making ongoing efforts to maintain contact with past participants. Not only does this communication allow for the collection of longitudinal data for evaluation purposes, it provides ongoing encouragement to these students to support their future success, and it keeps doors open for possible future collaborations, program recruitment, and professional network building. Looking ahead, the MRSEC will establish a centralized mechanism for more formal, ongoing communications with its past and future REU students, as well as its graduate student and post-doctoral members.
**Plans for the next reporting period:** The Center for Nanoscale Science will continue to emphasize and prioritize both established and newly initiated efforts to recruit and retain broad participation in its research, outreach, and educational activities. The Center’s key strategies for the coming year are as follows:

- Implement the two new diversity initiatives outlined within the renewal proposal (Sloan Scholars partnership to bring diverse graduate students into Center research activities, and the MRFN (Faculty) Speaker Series to invite external diverse faculty to visit the Center and explore potential research collaborations).
- Maintain active involvement and participation by Center faculty and staff in the university-wide Fall STEM Open House (for prospective diverse graduate students and senior year REU students) via hosting tours and interviews, networking, and serving as panelists and speakers.
- Continue to hold regular meetings of the MRSEC Diversity Committee and expand its connections and communication with all stakeholders: Center faculty, college diversity officers, graduate admission committees, and REU program leaders within the interdisciplinary departments and colleges associated with the MRSEC.
- Strengthen Center representation at individual department and college level graduate recruitment, admissions, and retention activities (via service on grad recruitment committees to build direct connections between departmental diversity efforts and the Fall STEM Open House).
- Further identify, establish, develop, and foster effective contacts and connections with programs and institutions that are dedicated to the advancement of underrepresented groups in science, in addition to Meyerhoff.
- Encourage engagement by the entire MRSEC membership in efforts to both recruit and retain diverse graduate applicants.
- Continue to actively support and directly participate in the Penn State’s Millennium Scholars program by attending activities, providing mentorship, and hosting first year summer research opportunities via MRSEC projects.
- Continue to implement and support programs and initiatives that target female involvement in STEM fields, careers, research opportunities, and Center activities at all stages along the career path.
- Continue to strengthen the collaborative outreach and education partnership that is currently developing with the Materials Research Institute as a result of its new state-of-the-art research facility; utilize this partnership as an opportunity to attract, support, and retain underserved minority and female students, postdoctoral fellows, research associates, and faculty.
- Continue to support and lead efforts to increase underrepresented and underserved participation in K-12 science outreach and education programs (Science Leadership Camp Scholarships, High School Leadership Conference for Hispanic students hosted by the Society of Professional Hispanic Engineers, Upward Bound Math and Science programs via Arts Fest and SEECos).
- Establish an improved system for tracking and communicating with past MRSEC members, and actively involve these individuals in recruitment, retention, and professional development networking activities.
9. Knowledge Transfer to Industry and Other Sectors

The faculty of the Penn State MRSEC are engaged in a broad spectrum of activities with scientists and engineers in corporate and government laboratories within the U.S., and in exchanges and collaborations with international academic partners. These interactions include research collaborations, presentations at workshops and conferences, patents and software. The MRSEC hosts visiting scientists and plays a key role in the overall industrial/technology transfer infrastructure of the University. There is also strong international component to collaborative research and outreach activities of the Center.

Penn State is a significant performer of industry sponsored research and as such maintains research relationships with companies and national laboratories across diverse fields. Slightly over one year ago (i.e. in 2012), Penn State implemented an innovative new policy whereby the university does not assert ownership of intellectual property that issues from industrially-sponsored research. Penn State considers the net present value of the interactions and relationships that our faculty and students have with industrial professionals to be greater than the apparent future value of the proceeds from such IP. This policy has begun to further facilitate academic-industry partnerships in 2013 and beyond.

One of the important vehicles for collaboration with industry is the MRSEC’s Industrial Affiliates Program, now in its sixth year. Under this program, industrial sponsors become affiliate members of the Center by executing a sponsored research projects agreement and making a commitment to support sponsor MRSEC research at a minimum level of $25,000 annually, representing approximately half the cost of a graduate student researcher. Matching support for the student is provided by the Center. Students and faculty mentors serve as Center liaisons to each affiliate member, while working on a research project of mutual interest. Ongoing communication between the affiliate member, the students and supervising faculty members are expected. Scientists and engineers representing affiliate members may co-direct student thesis research, and Center students also serve in internships with affiliate members. The Center also provides fellowships for scientists and engineers representing affiliate members.

Research Collaborations with MRSEC Faculty, Workshops, and Faculty Presentations

Venkat Gopalan is working with Kodak on ferroelectric devices, and Susan Trolier-McKinstry works with IBM, Xaar, and Dow, on piezoelectrics related to IRG1 research. Long-Qing Chen works with the Ideal Semiconductor Company. In IRG4-related work, Professor Theresa Mayer works with Lockheed Martin Corporation on innovative electromagnetic structures.

MRSEC Personnel in the Seed effort on 2D materials organized a workshop “Graphene and Beyond” which took place in March, 2013 with attendees from industry, national labs, government, and academia. The Seed effort also worked with Kyna Technology, a small business, to develop large-scale Sulfur/Selenium ion exchange process, and presented MRSEC-supported research results at an invited talk at the International Symposium on Advanced Nanodevices and Nanotechnology, the Army Research Lab, and the 2013 Nelson W. Taylor Seminar in 2013.

In addition to other international visitors, IRG2 hosted visitors from the University of Dundee for collaboration on acoustically powered nanomotors and micromotors.

Industrial and National Lab Fellowships, Internships, or Employment:

Jessica Leung is currently working in Northrop Grumman. Ryan Pavlick received a Ph.D. and is currently working at the Intel Corporation, as is Samudra Sengupta. Justin Sparks received a
Ph.D and is currently working at Dow Chemical. Hua Zhang received his Ph.D. and is currently working at Lubrizol Corporation.

(Cross-referenced to international activities) Qing He, a postdoc in 2013, is currently a professor at Durham University in Scotland. Che-Hui Lee received a Ph.D in 2013 and is working in Taiwan. Thomas Lummen, a postdoc in 2013, is currently a staff member at EPFL, Lausanne. Wei Wang received a Ph.D and is currently an Associate Professor of Materials Science, Harbin Institute of Technology, Harbin, China.
10. International Activities

The Penn State MRSEC has a substantial international component to its research and outreach program. The fiber-based research program in IRG4 benefits from a deep and long-term relationship with the University of Southampton, with provides critical expertise on the fabrication of the fiber platform. In addition, IRG3 has strong connections to China, particularly since several alumni of this IRG3 have recently taken up permanent positions there. IRG2’s work on ultrasomically powered motors is proceeding in part through interactions with collaborators in France and Dundee. IRG1 also has several important relationships with international collaborators. Specific international activities in the past year include the following:

- Tony Huang presented IRG2 research at the International Conference on Optofluidics in Hong Kong and at an Optofluidics Workshop in Xi’an, China in August 2013. He also presented at Malvern Instruments Inc. in Malvern, at the 2013 International Acoustofluidics Conference in Southampton, and (on Lab-on-a-Chip Technologies Enabled by Acousto-Opto-Fluidics) at the University of Dundee and the University of Glasgow in the UK, in September 2013

- Chao-xing Liu presented IRG3 research in an invited talk at the Topological Materials workshop in Sanya, China in December 2013, and also an invited talk at the 16th International Conference on Narrow Gap Systems in Hangzhou, China in August and the International Workshop on Unconventional Superconductivityat Jiaotong University, Shanghai in May.

- Jainendra Jain and his student Ajit Balram visited the Indian Institute of Science, Bangalore, for two months in 2013, and Professor Jain was featured on a "Meet a Scientist" show sponsored by Education Satellite Program in the Indian State of Punjab, broadcast to students >1000 rural high schools.

- Qi Li in IRG3 maintains collaborations with Professor X. G. Li's group at the University of Science and Technology of China; Professor Li is a guest professor at USTC.

- Professor Theresa Mayer in IRG4 gave a seminar at École Polytechnique de Montréal, Montreal CA in October 2013.

- Professor Werner in IRG4 collaborated with the Electromagnetics Group at the University of Granada, Granada, Spain to develop efficient computational modeling techniques for nanowire antennas, carbon nanotubes and graphene. He also gave an invited seminar on Transformation Optics at the University of Trento, Trento, Italy.

- Mauricio Terrones, an investigator in the Seed program, hosted two visiting faculty (Prof. Ignacio Martin-Gullon & Dr. Esther Asedegbega) and two graduate students (María Crespo and Claire Antonelli) from Spain to contribute to the work of defective 2D systems. In addition, Professor from Brazil, Maria Cristina Dos Santos visited the MRSEC to work on the interactions of 2D systems with different molecules. Prof. Bartolomeu Viana visited from Brazil to work on the synthesis and Raman characterization of 2D systems.

- Professor Terrrones gave numerous invited international seminars, at INCAR, Oviedo (Spain); Universidad Autónoma in Madrid; Graphene Brazil 2013 in Rio De Janeiro; IM-
DEA-Materials, Madrid, Bremen, Germany; Sendai, Japan, and at the 4th Mexican Workshop on Nanostructured Materials, held in Puebla, Mexico.

- Qing He, a postdoc in 2013, is currently a professor at Durham University in Scotland. Che-Hui Lee received a Ph.D in 2013 and is working in Taiwan. Thomas Lummen, a postdoc in 2013, is currently a staff member at EPFL, Lausanne. Wei Wang received a Ph.D. and is currently an Associate Professor of Materials Science, Harbin Institute of Technology, Harbin, China.
11. Shared Experimental and Computational Facilities

The MRSEC is closely integrated with the facilities of the Penn State Materials Research Institute (MRI), which include the Penn State Nanofab, the Materials Characterization Laboratory (MCL) and Materials Simulation Center (MSC). This integration and coordination ensure that MRSEC’s investments in fabrication, characterization and computation have maximal institutional impact. MRSEC faculty provide the leadership for certain of these facilities, with Theresa Mayer serving as the Director of the Penn State Nanofabrication Laboratory (note that the situation as regards the nation-wide NNIN program is currently in flux). The MRSEC also works closely with the management of the MCL particularly as regards the MFRN effort and in the acquisition of major new equipment. The synergistic relationship among the MRSEC and these three user facilities also ensures that the strategic directions and investments of the core facilities are mutually beneficial and beneficial to the MRSEC research and educational missions. The MRSEC Central Facility Laboratory (CFL) dovetails with the MRI facilities, providing specialized instrumentation that primarily serves the research needs of the Center. All three user facilities are not only integral to the MRSEC research programs, but are also integrated into the MRSEC Summer REU/RET, the Materials Research Facilities Network, as well as other outreach programs that serve middle school girls, teacher workshops, and at-risk youth.

Both the Nanofab and MCL are cost recoverable user facilities with rates defined on the basis of maintenance, repair and staffing in accordance with federal cost-accounting procedures and are reviewed annually by the Office of the Corporate Controller. Both facilities are operated by professional full-time staff, who coordinate numerous educational and training activities which are highly integrated into formal courses offered by Penn State faculty. Beyond providing administrative leadership, MRSEC investigators play key roles in transferring cutting-edge research techniques to these widely accessible user facilities. External outreach is accomplished via several means, including Penn State’s node of the NSF National Nanotechnology Infrastructure Network (NNIN), which supports professional staff who serve as liaisons with external industrial and academic users and also by the Materials Research Facilities Network. MRSEC faculty provide input into strategic planning for the fabrication and characterization facilities through faculty steering committees and focus groups centered around specific types of instrumentation or processes (e.g. optical spectroscopy, lithography, electron microscopy).

The MRSEC also helps to support the Materials Simulation Center (MSC), a University-wide facility providing education, support and research activities to help users incorporate simulation into their research programs, through regular contributions towards computational hardware. The MSC sponsors short courses and workshops on simulation/modeling software on a regular basis. The MSC also hosts regular user group meetings organized around particular types of simulation, including, the Density Functional Theory User Group and the General RCC & MSC User Group. An effective sharing system managed and supported by RCC and the MSC helped MRSEC users to take advantage of the full potential of the whole cluster and resulted in numerous findings and publications with the help from MSC/MRSEC.

The MRSEC Central Facilities Laboratory (CFL) is comprised of several laboratories that contain instruments for advanced electrical and optical characterization and sample preparation. The low-temperature characterization facility is a unique user facility in the MRSEC network and houses a physical properties measurement system (PPMS) that allows for electrical transport and heat capacity measurements from 400 K down to 50 mK and under fields as high as 9 T,
a $^3$He-$^4$He dilution refrigerator (12 mK to 400K, up to 9T), and a micromanipulated probe station (4-450 K; up to 3T). CFL facilities are available to other internal and external users, but are managed and funded directly by the MRSEC. Moses Chan provided overall coordination of the CFL. The Executive Committee reviews the CFL operating policies and budget on a regular basis. The MRSEC Executive Committee also reviews and prioritizes equipment requests from the IRGs on an ongoing basis.

Several equipment acquisitions have supported MRSEC research in addition to the wider materials community, including: (1) A gas injector, gas inlet system and high temperature effusion cell including controller and power supply installed in an MBE system and for efforts such as aluminate thin film growth with hybrid MBE that can test IRG1 predictions on hybrid improper ferroelectricity (made by Rondinelli and Fennie). (2) Lenses and fast cameras for the Olympus BX60M optical microscope located in Chemistry Room 219 and are accessible to all MRSEC users, with on-site training. The camera's uses include the investigation of the ultrafast motion of nano- and micromotors to shed light on mechanistic details of propulsion and rotation of motors. In addition to high temporal resolution, the camera also has high spatial resolution which enables a more precise determination of nano- and microparticle size and shape and hence a correlation of these properties with motor motion. (3) A Vytran glass processing system with WCS-3000 and GPX-TMS options was purchases for splicing capillaries to serve as high pressure chemical reactors and to draw down micro capillaries into nano- capillaries to serve as templates for the fabrication of ultralong nanowires, of use in IRG3 and beyond. (4) An Andor SR-303i-B spectrometer and DU 420A-BEX2-DD detector are being used to measure the optical response of nanoparticles and optical devices of interest to IRG4. It is located in N-226A MSC building and accessible to potential users both within and outside the MRSEC.

As a member of the Materials Research Facilities Network our primary goal in administering our Faculty Fellow program is to catalyze and support access to advanced characterization, fabrication and computational resources by researchers from primarily undergraduate institutions. Pennsylvania has a significant number of colleges and universities (>250) and Penn State being strategically located in the center of the state affords a unique opportunity to serve these researchers. The Penn State program has been optimized to provide the highest impact in light of the opportunities unique to our site. In 2013 five fellows were supported: Kofi Adu (PSU Altoona), Rose Clark (St. Francis University), Alison Noble (Messiah College), Sarah St. Angelo (Dickinson College), and Marian Tzolov (Lock Haven University). Additionally, these faculty often brought undergraduate researchers working on their respective projects to Penn State to participate in fabrication and analyses. This not only helped to advance the research but also served to broaden the horizons of these students. In light of the fact that all of the 2013 fellows are within driving distance to the University Park campus they continue to access the facilities throughout the academic year.
Kofi Adu, an Assistant Professor of Physics at Penn State Altoona performed a project “Synthesis of MgB2 Nanowires to Investigate Strain Induced Effect on the Superconducting Critical Temperature” with the goal to synthesize MgB2 nanowires and perform structural and morphological characterization. Nanowires are synthesized via a vapor-liquid-solid (VLS) mechanism. SEM and TEM reveal a low concentration of nanowires being grown using the current approaches as well as the formation of some “sheet-like” species. As such, there is a need to increase the deposition temperature to increase the yield of nanowire species. This work is ongoing. Quote: “The benefits of the program to me as a fellow are four fold: (1) as an experimental condensed matter physicist, the program provides the opportunity to gain materials characterization skills using the plethora of characterization instruments that the MCL of MRI at Penn State offers, (2) the data that will be acquired during the program will be published in a peer review journal thus, contributing to my career development, (3) as a tenure-track faculty, this program will help bolster my bid for tenure, and (4) the program exposes the undergraduate student(s) working with me to the state-of-the-art instrumentations as core part of their undergraduate education, providing them with hands-on training and strengthening their interest in pursuing materials research in graduate school.”

Alison Noble an Assistant Professor of Chemistry at Messiah College performed a project “Self-Assembled Monolayers on ZnSe: SAM / Liquid Crystal Thin Film Interactions” with the goal to study surface morphology and chemical nature of mechanically polished ZnSe substrates as well as the chemisorption of thiolate and carboxylate SAMs on ZnSe. It was determined that the ZnSe cleaning protocol (UV-O3) alters the near surface chemistry to create a significant oxide layer. The formation of this oxide layer may significantly impact the formation, density, and orientation of SAMs on the surface. Additionally cleaving of a ZnSe crystal and measurement of the fresh fracture via XPS revealed that under standard conditions ZnSe forms an oxide. Work is ongoing. Quote: “Access to the advanced instrumentation and interaction with the knowledgeable staff at PSU has been critical to the success of this project. Because of the flexibility of the MRFN program, I was also able to actively include undergraduate students from my home institution in the work, providing them an opportunity to use advanced instrumentation and collaborate in meaningful interdisciplinary research. The staff members at MCL are professional, helpful, and knowledgeable experts.”

Rose Clark a Professor of Chemistry at St. Francis University performed a project “Understanding the Electrochemical Response of Small Molecules at a Mixed Self-Assembled Monolayer: Probing the Surface Topography and SAM/Au Structure” with the goal to characterize and better understand the surface structure of three different gold electrode surfaces and the monolayers formed on these surfaces. Difference observed in the electrochemical response of these surfaces has prompted the need for additional characterization. AFM work performed to date clearly demonstrates a difference in the surface topography of the three gold electrode surfaces (as purchased, flame annealed, and evaporated Au). Additionally, anomalous surface deposits were observed on the surface of samples leading to a modification of the cleaning protocol used prior to SAM deposition. FTIR analyses were performed on SAMs formed on the surface of the Au film deposited by thermal evaporation. It was concluded that disorder monolayer formed under all assembly conditions. Quote: “The partnership with PSU has been wonderful to address the important surface topography questions due to the surface characterization capabilities available. The data collected at PSU with the help of the MRFN grant has provided a much clearer picture of our electrode surfaces. The staff at MCL have been great and have gone out of their way to find time to work on the project.”
Sarah St. Angelo, an Assistant Professor of Chemistry at Dickinson College, performed a project “Characterization of Cu, Cu oxide, Ag, and Au Nanoparticles Reduced with Plant Teas” with the goal to characterize the metal, metal-oxide, and mixed metal nanoparticle/nanoplates synthesized via methods involving teas made from lemongrass stalks or ginko leaves. UV-Vis, Raman, and fluorescence techniques are used at Dickinson College but there is a need to understand the structure/chemistry of these particle via TEM. TEM has shown that Au particles of three types being formed by the ginko reduction process: spherical ~5 nm particles, ~20-50 nm facetted spherical particles and triangular platelets. It was found that the ~5 nm spherical particles could be isolated via centrifugation. The observation of various sizes/shape nanoparticles supports optical absorption data collected at Dickinson which shows multiple absorption peaks. Work is ongoing. Quote: “Dickinson is a small liberal arts college that does not have a graduate program, so our research schedule is greatly affected by the undergraduate academic schedule. Also, we do not have the suite of characterization techniques necessary to fully participate in nanoparticle research. The MRFN Faculty Fellows program at Penn State University has provided me with an exceptional opportunity to conduct my research in the world-class Millennium Science Complex, to access instrumentation and technical expertise that are unavailable at my home institution, and to augment my own understanding of my research field. The data I have been able to obtain through this program will improve my chances of publishing my work in a high quality journal.”

Marian Tzolov, an Associate Professor of Physics at Lock Haven University, performed a project “Structural studies of zinc oxide nanowires and zinc tungstate films” with the goal to acquire structural information about zinc oxide nanowires and zinc tungstate thin films using XRD and TEM to complement SEM and AFM data acquired at Lock Haven. XRD of the ZnO revealed very useful information which lead to a better understanding of the current deposition process, specifically that a preferential film orientation is induced when carbon monoxide is used during growth. XRD was also useful in confirming the structure of the zinc tungstate thin film. TEM work thus far has revealed a variety of nano-scale species in the ZnO reaction products which include: gels, belts, and nanowires with catalyst in place. Quote: “The idea of giving access to the unique equipment at PSU to faculty from other institution who have an active research program is a very efficient way to utilize the equipment and to stimulate research. I see the efficiency in several aspects: (a) ensuring higher use of the equipment; (b) preventing acquisition of equipment at other institution with will be not of this good quality and not so well utilized, maintained, and supervised; (c) lowers the barriers between the institutions and stimulates contacts.”
12. Administration and Management

The organizational structure of the Center is outlined in the chart at right. Daily operations are managed by the Director, Vincent Crespi, who reports directly to the Senior Vice President for Research. Center policy is developed by consultation of the full membership and is implemented by its Executive Committee. The committee currently consists of the Director Crespi, the Associate Directors Mallouk and Chan, the IRG leaders (Gopalan, Sen, Chan and Mayer), the Penn State Materials Research Institute (MRI) Director Carlo Pantano, Outreach Director Dreyer and Mohney. Mallouk oversees the outreach portfolio. The Executive Committee is well connected to University administration in materials research through Pantano and Mayer (who is also Director of the Penn State Nanofabrication Facility), and all members of the Executive Committee are also active in the research and/or outreach activities of the Center. Mallouk and Mayer also serve on the MRI advisory board, further connecting the leadership of the Center and MRI. The Executive Committee meets approximately bimonthly, typically after the weekly MRSEC Seminar. While the scientific direction of the Center grows in a “bottom up” way by soliciting the most compelling research ideas from the full membership, the Executive Committee plays an important role in coordinating the review of new proposals and existing projects and ensuring that the research portfolio undergoes continual renewal. The Executive Committee is also charged with deciding resource allocation for facilities, coordinating the response of the Center to new initiatives from NSF and within the University, and guiding major initiatives in industrial outreach, educational outreach and international programs.

The full membership of the MRSEC meets weekly on Mondays at the MRSEC Seminar. These well-attended lunch seminars are a regular forum for reviewing scientific progress, introducing new ideas and new members, advertising outreach opportunities, performing career development activities with students and postdocs, and forming collaborations with visitors. They are also a natural place to communicate issues that are discussed in the Executive Committee with the members of the Center. In addition to these seminars, the students, postdocs and faculty in each IRG meet approximately bi-weekly to discuss their current research progress and challenges in more detail. Usually, at least one member of the Executive Committee is engaged in the research project and is present at those meetings.

The Center has a strong commitment to diversity, and successfully includes women at all levels. The MRSEC Diversity Committee, which includes the directors of diversity-focused initiatives in several Colleges, helps to coordinate recruitment at campus-wide. Members of the Diversity Committee include Mallouk (Associate Director and Chair), Ron Redwing, Francelys Medina (Educational Outreach Coordinator), Kristin Dreyer (Educational Outreach Manager), Hank McCoullum (Divinity Coordinator for the Eberly College of Science), Catherine Lyons (Associate Dean of Educational Equity for the College of Earth and Mineral Sciences), Mary Beth Williams (Graduate Admissions chair, Department of Chemistry), and Joan Redwing (MRSEC faculty and Graduate Admissions chair, Department of Material Science and Engineering). The
diversity committee has spearheaded a new university-wide STEM Open House graduate recruiting, the first offering of which took place in 2013.

The External Advisory Committee comprehensively reviews our programs and provides a vital mechanism of frank, critical, external feedback. The Committee is composed of experts in target areas (all IRGs, Educational Outreach, Industrial Outreach). Current membership includes John Brady (Caltech), Frank DiSalvo (Cornell), Vladimir Shalaev (Purdue), Orlin Velev (NC State), and Dragan Damjanovic (EPFL); committee composition is currently turning over due to term expirations and changes in focus of the IRGs. In several instances, visits of our Advisory Board have resulted not only in valuable advice to the Center but also to productive collaborations and industrial connections, as well as sharing of best practices for facilities and outreach.

The Executive Committee oversees the IRGs and Seed projects of the Center, and through a competitive review process decides on how support will be allocated. **Resources for research** are allocated in a manner that is intended to maximize innovation, productivity, and collaboration. Within IRGs, funds are not distributed to individual faculty, but instead support students and postdocs who work on multi-investigator projects. This organizational scheme is reflected in the internal accounting in that cost centers are not allocated to individual faculty, but instead to IRGs as a whole with centralized appointment of students. A similar policy is applied to projects within IRGs and Seed projects: in a sense, every project in the MRSEC is a Seed. Students are often jointly advised by faculty. Postdocs, who typically number 1 or 2 per IRG, are expected to play a broader collaborative role than graduate students, acting as a scientific “glue” across an IRG. Faculty (with the exception of the Director and Associate Directors) receive no salary support from the Center, although some are granted release time by their Departments. Faculty who are not the official thesis advisors of students on a particular project typically collaborate and often co-advising. The regular IRG meetings (and smaller ad hoc meetings of individual projects) promote these kinds of interactions. When projects are phased out of the MRSEC, care is taken to minimize the impact on the students involved to facilitate optimal career development. Because this system does not allocate funds to any particular faculty member, there is relatively little inertia to impede the inclusion of new faculty or the support of particularly promising new ideas in the IRGs. This flexibility has helped the IRGs change their course in response to new findings and challenges – historically, several IRGs have entirely renewed their research agenda via incorporation of especially successful Seed projects, for example. Many of the faculty are members of more than one IRG, and this confers synergy to the research projects.

The MRSEC has recently refocussed the current IRG Seed to focus on magnetic phenomena in 2D systems. The process of preparation for the renewal competition took place through early and mid 2013. A call was placed university-wide via a pair of Town Hall meetings in January 2013 for new IRG proposals. Nice potential IRG teams competed for slots in the renewal proposal, with ~50 external reviews solicited in spring/summer 2013 followed by a down-select.

The Center has a collaborative role with three **Institutes at Penn State** (MRI, the Huck Institutes for the Life Sciences, and the Penn State Institutes for Energy and the Environment) in reviewing and supporting Seed Projects. The Institute directors (Carlo Pantano, Peter Hudson, and Tom Richard, respectively) participate in the review process, and the Institutes co-fund appropriate projects of mutual interest and high intellectual merit. The web-based submission and review process is modeled after Fastlane, with the Executive Committee and Institute directors providing written reviews and later meeting as a panel to select projects for support. This is a win-win arrangement for the Institutes and the Center. The Center is able to leverage substantial addition-
al support for new projects and obtain review input from outside experts. The Institutes benefit from the broad competitive proposal solicitation and review, which historically has attracted 15 to 20 collaborative proposals from the Penn State materials research community. Projects selected in this process have generally been very successful, either as future IRG projects or as the beginning of multi-investigator collaborations that later become NIRTs, MURIs, or other major grants. In 2013, there was not a general Seed call, since the MRSEC is currently directing Seed resources towards the recently-funded IRG Seed.

**Educational outreach** is a strong unifying theme in the Center. Participation is expected of all students and postdocs and is encouraged from all faculty. Our educational activities are overseen by Associate Director Tom Mallouk. Dr. Ronald Redwing, a prior Outreach Director in the Center, is now an Associate Dean at Penn State, although he maintains an active interest and involvement in recruiting members of underrepresented groups for the MRSEC REU program and also spearheaded the new STEM Open House initiative in partnership with the MRSEC. Kristin Dreyer is Outreach Director. Postdoctoral fellow Francelys Medina is an educational outreach coordinator in the Center, currently specializing in the RET/REU program. Kristin Dreyer is the administrative point of contact for our collaborations with the Franklin Institute.

**Industrial outreach**, including workshops, personnel exchange, and joint support of students is overseen by Pantano, together with David Fecko, who oversees industrial outreach within the Materials Research Institute and reports directly to Carlo. Fecko was recently added to the Executive Committee.

Center operations, including budgets, subcontracts, reports, site visits, seminars, website maintenance, and appointment of personnel are managed by full-time administrative staff, Denise Patton. Financial reports and budgets are coordinated with the Grants Office in the Eberly College of Science and with the University Office of Sponsored Programs.
13. List of Ph.D students and postdocs graduating in 2013

Paul Browning will be receiving a Master’s Degree Spring 2014.

Charles Brooks received a Ph.D in 2013 and is currently a postdoc at Cornell for Darrell Schlom.

Qing He, a postdoc left in 2013 and currently a professor at Durham University in Scotland.

Che-Hui Lee received a Ph.D in 2013 and is working in Taiwan.

Jessica Leung received a Masters and is currently working in Northrop Grumman.

Thomas Lummen, a postdoc left in 2013 and is currently a staff member at EPFL, Lausanne.

Frank (Farhad) Namin received a Ph.D and is a faculty member in the Department of Electrical Engineering at Amirkabir University of Technology (Tehran Polytechnic, Tehran, Iran)

Ryan Pavlick received a Ph.D. and is currently working at the Intel Corporation.

Samudra Sengupta received a Ph.D and is currently working at Intel Corporation.

Justin Sparks received a Ph.D and is currently working at Dow Chemical.

Wei Wang received a Ph.D. and is currently an Associate Professor of Materials Science, Harbin Institute of Technology, Harbin, China.

Hua Zhang received his Ph.D. and is currently working at Lubrizol Corporation.
14. Publications and Patents

IRG 1

A. Primary


B. Partial Support


C. Shared Facilities
None

IRG 2
A. Primary Support


**B. Partial Support**


**C. Shared Facilities**

None.

**IRG 3 (Chan)**

**A. Primary Support**


B. Partial Support


C. Shared Facilities

None.

IRG 3 (New - Badding)

A. Primary Support

None.

B. Partial Support


IRG 4
A. Primary Support


X. Wang, D. H. Werner, and Jeremiah P. Turpin, “Investigation of Scattering Properties of Large-Scale Aperiodic Tilings Using a Combination of the Characteristic Basis Function and


**B. Partial Support**


C. Shared Facilities

None.

SEED

A. Primary

None

B. Partial


C. Shared Facilities
none

**Patents**

**IRG 1 – none**

**IRG 2**

Tony Huang, Acoustofluidic micro mixer, (U.S. Filing, PSU Invention Disclosure Number 2013-4103, PST-71018/36)

Tony Huang, A Reconfigurable Plasmofluidic Lens, (U.S. Patent Filing)

Tony Huang, Continuous Enrichment of Low-Abundance Cell Sample Using Standing Surface Acoustic Waves (SSAW), (U.S. Patent Filing, 61/891,010)

**IRG 3 (Chan) - none**

**IRG 3 (New - Badding)**


**IRG 4 - none**
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B.S.  1998  :  Metallurgical Engineering, Sharif University of Technology, Tehran Iran
M.S.  2001  :  Materials Science and Engineering, Worcester Polytechnic Institute
PhD.  2007  :  Materials Science and Engineering, Northwestern University
Postdoc  2012  :  Physics Department, University of California, Berkeley
2013–present  :  Visiting Scientist Fellow, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA
2008–2012  :  Post Doctoral Researcher, Physics Department and Center of Integrated Nanomechanical Systems, University of California, Berkeley
2002–2007  :  Graduate Researcher, Materials Science and Engineering Department, Northwestern University

Five products most closely related to the project

Five other significant products

Synergetic Activities  

Graduate Advisors and Postdoctoral Sponsors
Dr. Vinayak Dravid (Northwestern), & Dr. Alex Zettl (University of California Berkeley).
Five products most closely related to the project


Five other significant products


Synergistic Activities

(1) Member and former officer, U.S. National Academy of Science. (2) Member, American Academy of Arts and Science. Fellow, and former Executive Board Member, of the American Physical Society. (3) Wrote four graduate textbooks in physics: Many-Particle Physics, Applied Mathematics, Quantum Mechanics in a Nutshell, and Condensed Matter in a Nutshell.

Graduate Advisors and Postdoctoral Sponsors

Graduate Advisor: John J. Hopfield (UC Berkeley). Postdoctoral Sponsor: none to list.
16. Honors and Awards

We are delighted to report that Professor Fennie has been awarded a MaxArthur Fellowship, the so-called “Genius” award, in 2013 for his work on multiferroics, with specific citation of the work that has been supported by IRG1.

We also note that Professor Long-Qing Chen was named Materials Research Society Fellow and Professor Roman Engel-Herbert received an NSF Career Award in 2013. Roman Engel-Herbert also received the Rustum and Della Roy Innovation in Materials Research Award (in early 2014). Professor Joshua Robinson was named a Corning Faculty Fellow and a Miller Faculty Fellow, and he received an Oakridge Young Investigator Enhancement Award.

Professor Mauricio Terrones received the Lee-Hsun Lecture Award from the IMR-Chinese Academy of Sciences and was elected Fellow of the American Association for the Advancement of Science (AAAS). He was also appointed a Visiting Fellow of Trinity College at the University of Cambridge.

Zhi Hao Jiang received Honorable Mention and a Travel Grant from the IEEE Antennas and Propagation Society Student Paper Contest in July 2013.
The Franklin Institute science museum in Philadelphia and the MRSEC have a longtime partnership, which most recently resulted in a 5th museum show called Pocket Tech. At a training meeting in October 2013, this set of hands-on, interactive, visual demonstrations was distributed to 16 science museums nationwide in a variety of geographical and socio-economic areas. During 2014, this kit is expected to be seen by more than 100,000 visitors. MRSEC members provide content ideas, feedback during the development process, ongoing technical oversight, and supplemental fact sheets. AT&T augmented each kit with a refurbished smart phone.

Pocket Tech’s six demonstrations explore the technology contained within personal electronic devices. Real electronics and interactive models explain the notable software and hardware functions of pocket-sized computers: the binary language of data storage and processing, logic gates, color displays, screen re-orientation, touch screens, and wireless signal transmission. The activities build deeper understanding of this common technology, and provide insight into emerging areas of materials science and computational research.
To further increase the diversity of our Center, the Penn State MRSEC targets institutional-level change in pipeline issues of recruiting, support and retention. In addition to continuing effective diversity-focused efforts that have yielded female and URM representation consistently in excess of that in member departments, three new diversity initiatives were implemented in 2013:

• Fall STEM Open House for prospective graduate students and senior REU students.

• Joint series “Different People, Different Science, Working Together” with diversity training integrated with exposure to interdisciplinary research for participants in multiple summer research programs.

• Partnership with Penn State’s new Millennium Scholars program to match MRSEC faculty to first-year undergraduate scholars for their first summer research experience.
Chemical vapor deposition (CVD) is a mainstay of the semiconductor industry. Films of materials useful for chips, solar cells, displays, window coatings etc. are made in large and expensive reactors up to many meters in size. MRSEC researchers have developed a high-pressure CVD, which allows for conformal and void-free deposition of semiconductor films in much smaller and less expensive reactors that can deposit in much tighter spaces. For example, the interiors of optical fiber pores only microns to nanometers in diameter and nanoporous materials can be conformally coated and then filled completely because at high pressure molecules are only a nanometer apart.
MRSEC researchers have recently designed and demonstrated a broadband, polarization-insensitive metamaterial with greater than 98% measured average absorptivity over a wide ±45° field-of-view for mid-infrared wavelengths between 1.77 and 4.81 μm. This work represents a significant step toward realizing practical optical metamaterial absorbers that provide near-perfect broadband absorption over a specified super-octave bandwidth. The metamaterial absorbers were fabricated at the Penn State NSF NNIN site.
Piezoelectric materials convert electrical signals to mechanical motion. They are typically lead-based solid solutions that exhibit a “morphotropic” phase boundary: a region of intermediate composition separating two distinct phases where a new bridging phase with enhanced properties arises. The MRSEC team has shown that even simple perovskite ferroelectrics such as BaTiO$_3$ and KNbO$_3$ exhibit analogous “thermotropic” phase boundaries in wide temperature regions around thermal phase transitions. In these regions, new low-symmetry bridging phases arise that exhibit up to 400% enhancement in nonlinear optical and piezoelectric properties. These bulk phases are stabilized by long-range internal elastic and electric fields arising from a network of competing ferroelectric domains. A small symmetry breaking can thus greatly enhance physical properties.

Nature Commun. | 5:3172 | DOI: 10.1038/ncomms4172
Layered Ferroics as Superior Microwave Dielectrics

Penn State MRSEC DMR-0820404, DMR-1120296, IMR-0417392, Army Research Office: C-H Lee¹,², N. D. Orloff³,⁴, T. Birol⁵, Y. Zhu¹, V. Goian⁵, R. Haislmaier², E. Vlahos², J. A. Mundy¹, Y. Nie¹, M. D. Biegalski⁶, J. Zhang¹, M. Bernhagen⁷, N. A. Benedek⁸, Y. Kim¹, J. D. Brock¹, R. Uecker⁷, X. Xi⁹, V. Gopalan², D. Nuzhnyy⁵, S. Kamba⁵, D. A. Muller¹, I. Takeuchi⁴, J. C. Booth³, C. J. Fennie¹ & D. G. Schlom¹


IRG1 of the Penn State MRSEC, in close collaboration with the Cornell MRSEC, U Maryland, NIST and others, has designed and demonstrated the world’s best tunable microwave dielectric, operating with the highest reported figure of merit up to 125GHz. This achievement could result in a new generation of superior electronically tunable microwave filters, antennas, and phase shifters for improved wireless communications in cellphones and other devices. The team predicted an unusual polar state in Sr\textsubscript{n+1}Ti\textsubscript{n}O\textsubscript{3n+1} Ruddlesden-Popper phases under tensile biaxial strain, where beyond a critical layer number of layers \( n \) an in-plane polarization appears within the perovskite layers. These structures are believed to accommodate variations in composition through the formation of additional rock-salt SrO layers, thus significantly decreasing dielectric losses. Lead author Lee was supported by the Penn State MRSEC and received his PhD from Penn State in 2012. Haislmaier, Vlahos, and Gopalan performed nonlinear optical characterization.
A crack in a high mineral-content material, like bone or a synthetic mineral/polymeric composite, generates ion gradients which can be utilized for active targeting and repair: Active self-propelled particle-based detection, delivery, and repair of cracks uses the damaged matrix itself as both trigger and fuel. This approach augments current research, which promotes bone healing by delivering a therapeutic agent to the bone by passive diffusion, by introducing active transport of the healing agent to the site of the injury. This targeting mechanism was used to deliver a fluorescently labelled drug (sodium alendronate) loaded onto nanoparticles. The colorimetric assay measures increase in cell growth induced by the drug and confirms the delivery of an active agent and thus cell proliferation.
We recently developed small molecule reagents that can be grafted onto polymer beads or surfaces to create a variety of “smart pumps”. The bead pumps fluid when exposed to UV light, but then it continues to pump the fluid after UV light is removed: a self-propagating reaction keeps the pump operating even after the stimulus is removed. Thus, the bead/pump has a “memory” for the stimulus and is capable of responding even when the stimulus is fleeting. An attractive feature of this type of system is the ease with which we should be able to modify the chemistry of the reagents to enable the system to respond selectively to a variety of stimuli.
Patterning of nanowires in a controllable, tunable manner is important for the fabrication of functional nanodevices. MRSEC researchers have used standing surface acoustic waves to construct large-scale nanowire arrays with well-controlled patterning geometry and spacing within 5 seconds. By controlling the distribution of an acoustic field, metallic nanowires can be assembled into different patterns. This technique possesses several advantages over alternative patterning approaches, including high versatility, tunability, and efficiency, making it promising for a variety of device applications.
A Y-shaped microfluidic device generates a gradient in the concentration of “substrate,” the fuel for an enzyme. Both catalase and urease enzyme molecules move towards areas of higher substrate concentration, the first demonstration of chemotaxis by enzyme molecules. By using glucose oxidase and glucose to generate a hydrogen peroxide gradient, we also induce the migration of catalase towards glucose oxidase – a more complex sequence of chemical triggers. This control over the motion of individual molecules through chemical gradients mimics similar processes in biology and extends our ability to manipulate objects on the nanoscale.

*J. Am. Chem. Soc.*, **2013**, *135*, 1406
Silver phosphate micromotors reversibly transition between two collective behaviors by the addition and removal of NH$_3$: repulsive dispersion-like “exclusion” and attractive clustering-like “schooling”. Particles cluster hierarchically when other inert particles are also present. Upon the addition of NH$_3$, large Ag$_3$PO$_4$ microparticles function as pumps, pushing away inert particles from their vicinity. The transition from dispersion to clustering can be halted with UV light. By combining the two external stimuli, the micromotor system can be used as a logic gate, with UV and NH$_3$ stimuli as inputs and collective “schooling” and “exclusion” behaviors as outputs. This suggests their potential for application in autonomous chemical computation.

*J. Am. Chem. Soc.*, 2013, 135, 1280
Quantum tunneling events in superconducting nanowires

Penn State MRSEC DMR-0820404: Meenakshi Singh & Moses Chan

In quasi-one-dimensional nanowires, superconductivity is destroyed by phase slip events. Phase slips can be caused by thermal activation over a free energy barrier or quantum phase slip through the barrier (QPS). QPS, an example of macroscopic quantum tunneling, has not been unambiguously demonstrated because of the interference of thermal activation. In this experiment, the two processes are cleaning separated by the anti-proximity effect (discovered earlier by the MRSEC) where a phase-slip-free superconducting region is stabilized by the dissipative environment of the normal electrodes. Individual QPS events deep in the superconducting phase are detected by single-shot voltage measurement, in which they appear as stochastic switching events from the superconducting to the normal state.

PRB 88, 064511 (2013)
An extremely long Ga-In eutectic nanowire confined inside a hollow glass fiber of 150 nm inner diameter shows novel hysteretic switching between stable superconducting and resistive states. The nonzero resistance occurs when a Ga nanodroplet spontaneously formed along the length of the nanowire traps one or more superconducting fluxons, thereby driving a Josephson weak-link created by a second nearby Ga nanodroplet normal. This experiment opens the possibility of developing single-fluxon logic and memory devices.