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, ordered nanoscale metalattices, 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 Nanolithography (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. In 2014, the Center renewed again, with a new focus to IRG1 (layer tuning of ferroic properties), a rejuvenated IRG2, a new IRG3 focused on three-dimensional ordered nanoscale metalattices (produced using methods pioneered in the fiber efforts of the prior IRG4) and a new IRG4 focused on multicomponent assemblies designed for collective (and reconfigurable) electronic and/or optical functionality.

The four IRGs investigate emergent behavior of nanoscale systems with common themes of:

- **IRG1, Designing Functionality into Layered Ferroics**, 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 layer stacking, strain, 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. The team has demonstrated that ferroelectricity can emerge at scale is reduced, challenging long-held notions that is is inevitably suppressed in this regime. Oxynitrides have been produced at low temperatures and high quality, opening up a new material class to mixed anionic compounds. New principles in domain wall control have been developed, and hybrid MBE techniques have been developed to deposit wafer-scale vanadate films with exceptional control of valence state.
Executive Summary

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. The IRG team has recently demonstrated an ability to quench the Brownian orientation diffusion of nanometers so that they move in consistent directions for prolonged periods of time, using active quenching effects near boundaries. Prior advances in active pumping within dead-end pores is now being extended to pseudomorphic mineral replacement reactions, with potential application in industrial processes. Advances in enzyme and substrate gradient control in microfluidic chambers has enabled a clear quantification of the excess migration due to powered motion up gradients. In acoustic systems, new insights have been gained in the relative roles of shape and density of constituent metals, and new mechanisms of acoustic control over particles, cells and microorganisms has been gained through use of bubbles, excitable cilia-like structures, and periodic potentials. Finally, advances have been made in low-cost acoustic tweezers for potential use in diagnostics.

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 State Materials Research Institute (MRI) the Huck Institutes for the Life Sciences, and the Penn State Institutes for Energy and the Environment. In the past year the Center continued support of a Seed effort on 2D tunable magnetic semiconductors (phasing out) and ramped up support of Seeds on topological superconductivity and 2D GaN.

**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, 24 K-12 teachers, 27 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.

The museum kit *Pocket Tech*, which explores the technology contained within personal electronic devices, which was distributed to 16 science museums nationwide in late 2013, reached ~100,000 museum visitors in 2014. These demonstrations are hands-on, interactive, visual, and tactile. MRSEC members provided the initial inspiration and content ideas, feedback during the development process, ongoing technical oversight, and
Executive Summary

IRG3, High Pressure Enabled Electronic Metalattices is ramping up a new MRSEC effort in realizing high-quality three-dimensional ordered periodic arrays of semiconductors through high-pressure deposition. The team has now synthesized periodic arrays of silicon and germanium from ordered silica sphere templates as small as 14 nm, and has developed the ability to remove the template while preserving the metalattice against spontaneous collapse. Atomic layer deposition techniques have been developed to control interface properties, and fascinating results on photoluminescence in Si and Ge metalattices suggest that these systems are an ideal platform for elucidating the origins of light emission from Si and Ge. Joint theory/experimental studies are revealing important information about reaction kinetics for silane decomposition in these unusual thermodynamic conditions, and positron annihilation spectroscopy has established exceptionally complete filling of ordered templates. Ultra-low frequency Raman spectroscopy is revealing signs of nanoscale metalattice order, and theoretical studies have established that the metalattice platform can enable quantum confinement with highly dispersive electronic states, which also elucidating the importance of interfaces and strong suppression of thermal conductivity in metalattice geometries.

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 (>200 children and adults), Kids Day for the Central Pa Festival of the Arts (14 booths, ~1000 kids), 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 four Pennsylvania K-12 educators learned about nanoscale science and technology via a one-day workshop.

Center volunteers hosted a diverse group of 30 high school aged youth at the Science Leadership Camp, 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 continuation of the the STEM Open House (initiated by the MRSEC) and the Different Science, Different People, Working Together workshop at a campus-wide joint REU picnic, a partnership with the 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. In a major diversity highlight, the MRSEC partnered on four PREM proposals, two of which were successful.

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 eighth 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 approximately bimonthly, often after the Monday lunch seminars to discuss scientific progress of the various projects, review re-
quests for substantial resource allocation, and discuss optimal strategies to maintain constant growth and renewal of our research and outreach missions. The Executive Committee is paying special attention to the launch of the new IRGs associated with the NSF renewal, and also the new international component of IRG2.

The Penn State MRSEC is advised by an external Advisory Board, which will visit bi-annually, alternating with NSF-appointed site visit teams. A newly constituted Advisory Board will make its first visit in the year after the upcoming NSF second-year site visit. These 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). An ultrafast laser system has been upgraded to support work in IRGs 1, 3 and 4. Dual EELS and ion mill capabilities have been integrated into the advanced microscopy platforms at MCL, and shared Raman capabilities have been expanded and enhanced.

The Center supports a faculty fellow program that are intended to increase the participation of faculty and students from predominantly undergraduate and minority-serving institutions in the region. These activities leverage the full suite of characterization and fabrication tools available in the CFL and MCL.
2. List of Center Participants

Bioengineering (other engineering)
(i) Receiving Center Support
   none
(ii) Affiliated, not receiving Center Support
   Peter Butler; Full Professor
   yes

Chemical Engineering
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   Kristen Fichthorn; Full Professor
   no
   Darrell Velegol; Full Professor
   yes
(ii) Affiliated, not receiving Center Support
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Chemistry
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   Paul Cremer; Full Professor
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   Christine Keating; Full Professor
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   Thomas Mallouk; Full Professor
   yes
   Scott Phillips; Full Professor
   yes
   Ayusman Sen; Full Professor
   yes
   Raymond Schaak; Full Professor
   yes
(ii) Affiliated, not receiving Center Support
   John Asbury; Assoc. Professor
   yes

Electrical Engineering
(i) Receiving Center Support
   Suman Datta; Full Professor
   yes
   Chris (Noel) Giebink; Asst. Professor
   yes
   Zhiwen Liu; Full Professor
   yes
   Theresa Mayer; Full Professor/Assoc. Dean
   yes
   Douglas Werner; Full Professor
   yes
(ii) Affiliated, not receiving Center Support
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Engineering Science and Mechanics (other engineering)
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   yes
(ii) Affiliated, not receiving Center Support
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Materials Science and Engineering

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- Long-Qing Chen; Full Professor  yes
- Ismaila Dabo; Asst. Professor  yes
- Roman Engel-Herbert; Asst. Professor  yes
- Venkatraman Gopalan; Full Professor  yes
- Suzanne Mohney; Full Professor  yes
- Xiaoqing Pan; Full Professor  no
- Ramesh Ramamoorthy; Full Professor  no
- Joan Redwing; Full Professor  yes
- Joshua Robinson; Asst. Professor  yes
- James Rondinelli; Asst. Professor  no
- Darrell Schlom; Full Professor  no
- Susan Trolier-McKinstry; Full Professor  yes

(ii) Affiliated, not receiving Center Support
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Physics

(i) Receiving Center Support
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- Demetrios Christodoulides; Full Professor  no
- Vincent Crespi; Full Professor  no
- Craig Fennie; Asst. Professor  no
- Margaret Murnane; Full Professor  no
- Ying Liu; Full Professor  yes
- Mauricio Terrones; Full Professor  yes
- Jun Zhu; Assoc. Professor  yes

(ii) Affiliated, not receiving Center Support
- Eric Hudson; Assoc. Professor  yes
- Jainendra Jain; Full Professor  yes
- Chao-Xing Liu; Asst. Professor  yes
- Gerald Mahan; Full Professor  no
- Nitin Samarth; Full Professor  yes
- Jorge Sofo; Full Professor  yes

Other Science

(i) Receiving Center Support
- Jayatri Das; Non-Tenured Education Staff/Chief Scientist  no
  Franklin Institute (Education Outreach)

(ii) Affiliated; not receiving Center Support
none
### 3. List of Center Collaborators

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<th>Institution</th>
<th>E-mail</th>
<th>Field of Expertise</th>
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<th>Shared Facilities User</th>
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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 were re-defined in the competitive renewal process of 2014. The IRG portfolio was renewed through a robust internal competitive review, followed by successful transit through the NSF renewal competition. This process yielded two new IRGs and substantial redirection of two existing IRGs. The following provides a picture of the Center’s current activities.

**IRG1** focuses on 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. A recent re-focusing on exploitation of the layering degree of freedom is providing compelling new opportunities to exploit novel mechanisms to couple spin, charge and lattice degrees of freedom.

**IRG2** has focused 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 advances the fundamental understanding of nanomotor design to enable applications in the dynamical organization of nanomaterials and nanosystems, separations, sensing, actuation and biomedicine. Particular focus has been 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. New international collaborations have been established to bring in expertise in modeling and advanced acoustics.

**IRG3** aims to establish a new field of 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 (in the prior IRG4) and couples to unique high-harmonic coherent x-ray characterization techniques being brought into the MRSEC. As a pioneering effort in a novel class of materials, the initial stages of the effort are focusing on synthesis and property investigation (optical and transport) of high-quality samples from silicon and germanium deposition, with optimization of interfaces, degree of lattice order, choice of lattice geometry, and associated predictive theory.

**IRG4** is also a new effort, focused on the 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 within the MRSEC in the prior award period.

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. 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. The Center is supporting two compelling new Seed efforts in growth of III-V semiconductors (in particular, 2D GaN) on novel 2D substates and in the search for topological superconductivity in two-dimensional heterostructures (with support for a prior Seed on 2D magnetism winding down during the reporting period). These two efforts are seen as aligning strategically with future
opportunities in the area of 2D systems, and also in contributing towards diversity goals.

**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, 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 recruit at the high school level students both locally and from underrepresented groups in the Philadelphia area for the Science Leadership summer camp. A broad range of high schools and middle schools are 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. The STEM Open House, first offered in Fall 2013, grew substantially in 2015 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 University has just recently made an institutional commitment to substantially expand the Millennium Scholars program, which is a gratifying recognition of the MRSEC’s early support for the launch of this program.

The Center recruits students and postdocs from under-represented groups through ongoing collaborations with partner institutions, 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. Of four PREM proposals submitted with the MRSEC as partnerships, we were enthused to learn that two PREM partnerships were chosen for funding by NSF, and efforts to launch these programs effectively and build out these partnerships are continuing apace.
IRG1: DESIGNING FUNCTIONALITY INTO LAYERED FERROICS

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In this reporting period the IRG1 team has 33 peer-reviewed publications, including 1 each in Science, Nature Chemistry, and Nature Communications. Starting from its inception as a seed in 2006–2007, this group has published 226 peer-reviewed papers. This includes 21 in Nature and sister journals, 5 in Science, and 16 in Phys. Rev. Lett. The team has graduated 4 PhDs and 2 postdocs in 2014–2015.

The new IRG1 expands beyond strain as a tuning parameter and explores a rich variety of control knobs in layered complex oxides. In layered oxides (Figure 1.1, Ruddlesden Popper (RP), Aurivillius(AV), Dion-Jacobson(DJ), Perovskite Superlattices (PS)), additional design variables emerge in composition (species A, A’, B, B’), geometry (strain, octahedral rotations, bond angles), and topology (including layer connectivity as in RP, DJ, AV and PS, as well as layer dimensionality given by m,n), yielding a richer design space which can support new phenomena and superior properties. The goal is to design and discover fundamental new mechanisms and material classes of acentric oxides with strong coupling to spin, charge, and lattice degrees of freedom. The design idea is to design and control acentricity to couple to magnetism, charge and orbital ordering, and metal-insulator transitions. We propose new mechanisms in perovskite superlattices (PS) that create strong ferro functionalities from otherwise non-polar and highly distorted ABO₃ perovskites, thus vastly expanding the compositions available. The team’s expertise spans first principles and phase-field modeling predictions of new materials and phenomena, synthesis with unit-cell level precision, structural electrical, magnetic, and optical characterization, and prototype device demonstrations. IRG1 focuses on three areas in layered ferroics: (1) New Functionality and Couplings through Competing Interactions, (2) Expanding the Ferroic Design Space by Transforming Non-Polar Materials, and (3) Gradient-driven Ferroic Phenomena in Layered Structures. We have made significant progress in all these topics in the past year.

Design of New Layered Ferroics with Multifunctionality: Members of the IRG have published three review articles in this period. The first review article in Dalton Transactions (2021) (and a number of other recent theory articles) highlights recent theoretical and experimental studies that have shown how a combination of non-polar structural distortions in ABO₃ perovskites, commonly tilts or rotations of the BO₆ octahedra, can give rise to polar structures or ferroelectricity in several families of layered
perovskites. We discuss the crystal chemical origin of the polarization in each of these families – which emerges through a so-called ‘trilinear coupling’ or ‘hybrid improper’ mechanism – and emphasize areas in which further theoretical and experimental investigation is needed. We also consider how this mechanism may provide a generic route for designing not only new ferroelectrics, but also materials with various other multifunctionalities, such as magnetoelectrics, electric field-controllable metal-insulator transitions, and designing optical properties. A second review article in the *Annual Reviews* tries to capture the state of the art in computational approaches to formulate predictive structure-property relationships governing optical performance in a variety of inorganic materials. Detailed electronic structure analysis (ESA) in combination with avenues to disentangle structural and electronic contributions is shown to provide insight into the design of nonlinear optical materials and translation of ab-initio data into predictive models.

The IRG team has recently discovered several families of layered perovskites that exhibit improper mechanisms that our team has predicted over the past years. These include Ruddlesden-Popper phases such as $A$RTiO$_4$ (R=Rare earth ranging from La-to-Ho, $A$=Alkali) such as NaRTiO$_4$, and LiRTiO$_4$, to $(Ca, Sr)_{n+1}(Ti, Ru)_{n}O_{3n+1}$, Dion-Jacobsen such as $A'$LaBaO$_7$ ($A'$= Rb, Cs; $B$ = Nb, Ta), and double perovskites A$'$A'MnWO$_6$ such as PbMn(IV)TeO$_6$ and MnFeWO$_6$. Figure 1.3 shows a high pressure and temperature synthesis of MnFeWO$_6$ – a new magnetic and polar member of the AA'MnWO$_6$-type corundum derivative family. The crystal structure, non-centrosymmetry through optical second harmonic generation, magnetic phase diagram, and electrical and dielectric properties were revealed. First-principles calculations were carried out to better understand its structure, polarization, complex magnetic properties, and to point to new materials design with multifunctional properties. Many of the other works are in progress, and some are in the review or publication process.

In a collaborative effort (*Science*, 349(6254), 1314–1317 (2015)) involving U. Wisconsin, Penn State, and U. Nebraska, the team showed that a scale reduction leads to the emergence of ferroelectricity (at room temperature), challenging the long-standing notion that ferroelectricity is inevitably suppressed at the scale of a few nanometers. A combination of theoretical calculations, electrical measurements, and
structural analyses provides evidence of room-temperature ferroelectricity in strain-free epitaxial nanometer-thick films of otherwise nonferroelectric strontium titanate (SrTiO$_3$). We show that electrically induced alignment of naturally existing polar nanoregions is responsible for the appearance of a stable net ferroelectric polarization in these films.

The IRG1 team has also demonstrated the ability to tune the thermal conductivity of homoepitaxial SrTiO$_3$ films deposited by reactive molecular-beam epitaxy by varying growth temperature, oxidation environment, and cation stoichiometry (Figure 1.4). Both point defects and planar defects decrease the longitudinal thermal conductivity ($k_{33}$), with the greatest decrease in films of the same composition observed for films containing planar defects oriented perpendicular to the direction of heat flow. The longitudinal thermal conductivity can be modified by as much as 80% – from 11.5 Wm$^{-1}$K$^{-1}$ for stoichiometric homoepitaxial SrTiO$_3$ to 2 Wm$^{-1}$K$^{-1}$ for strontium-rich homoepitaxial $Sr_{1-x}TiO_x$ films – by incorporating ($SrO$)$_2$ Ruddlesden-Popper planar defects. (Appl. Phys. Lett. 107, 051902 (2015))

In addition to the oxides, oxynitrides have been explored extensively in the past decade, in particular because of their interesting properties, such as visible-light absorption, photocatalytic activity and high dielectric permittivity. Their synthesis typically requires high-temperature NH$_3$ treatment (800–1,300 °C)

![Figure 1.4: Tuning thermal conductivity via stoichiometry](image)

**Figure 1.4: Tuning thermal conductivity via stoichiometry:** Bright-field STEM images taken at different magnifications (a) and (b) of the film grown at 800 C. The excess strontium is clearly seen to form layers perpendicular to the growth direction. The dependence of longitudinal thermal conductivity in relation to film composition with excess strontium films showing the largest decrease. Appl. Phys. Lett. 107, 051902 (2015).

![Figure 1.5: A Ferroelectric with a Metal-Insulator Transition in BaTiO$_3$:N$_{0.4}$](image)

**Figure 1.5: A Ferroelectric with a Metal-Insulator Transition in BaTiO$_3$:N$_{0.4}$:** Two-step synthesis of oxynitride BaTiO$_3$:N$_{0.4}$. Perovskite BaTiO (oxide) converted to BaTiO$_3$:H$_x$ (oxyhydride) by CaH$_2$ reduction. BaTiO$_3$:H$_x$ is converted into BaTiO$_3$:N$_{2x/3}$ (oxynitride) by the low-temperature NH$_3$ treatment (this work), via the oxyhydride–nitride BaTiO$_3$:N$_x$:H$_x$. Ba, dark green; Ti, light grey; O, red; H, blue; N, light green. Here the lability of H in the oxyhydride allows H /N$^+$ exchange to occur by low-temperature ammonolysis (375–550 °C) to yield BaTiO$_3$:N$_{2x/3}$ via mixed O–H–N intermediates. The photos displayed below each structure show the color change of the specimens for $x = 0.6$. Compositions are approximated (left to right) as BaTiO$_3$ (Ti$^{4+}$), BaTi$^{2+}$O$_{2x}$H$_{0.6}$ (Ti$^{3+}$), BaTiO$_3$:H$_{0.18}$N$_{0.22}$ (Ti$^{6+}$) and BaTiO$_3$:N$_{0.4}$ (Ti$^{4+}$). The color change is related to the amount of Ti 3$d$ t$_2g$ electrons. Nature Chemistry 7, 1017–1023 (2015)
of precursors, such as oxides, but the highly reducing conditions and the low mobility of N$^3$– species in the lattice place significant constraints on the composition and structure—and hence the properties—of the resulting oxynitrides. The IRG team has a topochemical route (Figure 1.5) that enables the preparation of an oxynitride at low temperatures (<500 °C), using a perovskite oxyhydride as a host. The lability of H in BaTiO$_3$-xH$_x$ (x ≤ 0.6) allows H / N$^3$– exchange to occur, and yields a room-temperature ferroelectric BaTiO$_3$-xN$_2x/3$. This anion exchange is also accompanied by a metal-to-insulator cross-over via mixed O– H–N intermediates. These findings suggest that this ‘labile hydride’ strategy can be used to explore various oxynitrides, and perhaps other mixed anionic compounds. In addition, this work has yielded a multifunctional ferroelectric with a metal-insulator transition. (Nature Chemistry, 7, 1017-1023 (2015). doi:10.1038/nchem.2370)$^{17}$

Epitaxial strain is a powerful tool to induce functional properties such as ferroelectricity in thin films of materials that do not possess ferroelectricity in bulk form. The IRG1 team has stabilized the ferroelectric state in thin films of the incipient ferroelectric CaTiO$_3$ through the careful control of the biaxial strain state and the symmetry of TiO$_6$ octahedral rotations (Figure 1.6). Detailed structural characterization was carried out by synchrotron x-ray diffraction and scanning transmission electron microscopy. CaTiO$_3$ films grown on La$_{0.18}$Sr$_{0.82}$Al$_{0.59}$Ta$_{0.41}$O$_3$ (LSAT) and NdGaO$_3$ substrates experienced a 1.1% biaxial strain state but differed in their octahedral tilt structures. A suppression of the out-of-plane rotations of the TiO$_6$ octahedral in films grown on LSAT substrates resulted in a robust ferroelectric I$^m$mm phase with remnant polarization 5 mC/cm$^2$ at 10 K and $T_c$ near 140 K. In contrast, films grown on NdGaO$_3$ substrates with significant octahedral tilting showed reduced polarization and $T_c$. These results highlight the key role played by symmetry in controlling the ferroelectric properties of perovskite oxide thin films. (Applied Physics Letters, 106 219901 (2015))$^{18}$

Many applications of ferroic materials, such as data storage and spintronics, are achieved through the control and manipulation of their domain wall (DW) orientations and configurations. IRG1 researchers have proposed a rotational compatibility condition to identify low-energy DWs in perovskites with oxygen octahedral tilt instability. It is derived from the strong DW energy anisotropy arising from the rigidity and corner sharing feature of the octahedral network. This anisotropy can be described by the relation $K_{11} << K_{44}$, in the gradient energy coefficient tensor within the framework of the Ginzburg-Landau-Devonshire theory. We analyzed quantitatively the DWs in SrTiO$_3$ and explained successfully the unusual ferroelectric DW width and energy in BiFeO$_3$. We have also predicted a dramatic influence of the flexoelectric coefficients on the ferroelectric polarization reversal.$^{19}$ (Physical Review B, 2014. 90 (22) 220101). The team has also predicted unusual polar states in perovskite superlattices, including mixed

![Figure 1.6: Octahedral rotations and Ferroelectricity in CaTiO$_3$ films on different substrates:](image) STEM-HAADF and ABF images of (a) CaTiO$_3$/LSAT and (c) CaTiO$_3$/NdGaO$_3$ interfaces, viewed from the [010]$_c$ zone axis. Polyhedral models showing the octahedral tilts are overlaid on the images. The size bar is 1 nm. BO$_6$ rotation angle, b for (b) CaTiO$_3$/LSAT and (d) CaTiO$_3$/NdGaO$_3$ interfaces. Details in Applied Physics Letters, 106 219901 (2015).
Ising-Neel-Bloch type domain walls\textsuperscript{4,5} and ordered polar vortices.\textsuperscript{20} Indeed, we have recently experimentally demonstrated the presence of such ordered polar vortices in a PbTiO\textsubscript{3} / SrTiO\textsubscript{3} system, and the work is in print.\textsuperscript{20}

**Correlated Electronic Oxides:** The IRG team has developed hybrid MBE techniques to achieve the highest quality vanadate (VO\textsubscript{2}, SrVO\textsubscript{3}, LaVO\textsubscript{3}, CaVO\textsubscript{3}) thin films ever demonstrated,\textsuperscript{21,22} and on wafer scale (Figure 1.7) (Nature Communications 6, 8475 (2015)).\textsuperscript{23} Transition metal oxides offer functional properties beyond conventional semiconductors. Bridging the gap between the fundamental research frontier in oxide electronics and their realization in commercial devices demands a wafer-scale growth approach for high-quality transition metal oxide thin films. Such a method requires excellent control over the transition metal valence state to avoid performance deterioration, which has been proved challenging. To this end, the team has developed a scalable growth approach that enables precise valence state control. By creating an oxygen activity gradient across the wafer, a continuous valence state library is established to identify the optimal growth condition. Single-crystalline VO\textsubscript{2} thin films have been grown on wafer scale, exhibiting more than four orders of magnitude change in resistivity across the metal-to-insulator transition. Thus ‘electronic grade’ transition metal oxide films can be realized on a large scale using a combinatorial growth approach, which can be extended to other multivalent oxide systems. Using these films, we have recently demonstrated that electron correlation is a powerful knob that opens up correlated metals as a large new family of transparent conducting oxides. This work is in print, and will be elaborated on in the next reporting period (Nature Materials, 2015).\textsuperscript{24}
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13 "PbMn(IV)TeO$_6$: A New Noncentrosymmetric Layered Honeycomb Magnetic Oxide," Kim, Sun Woo; Deng, Zheng; Li, Man-Rong; Gupta, Arnab; Akamatsu, Hirofumi; Gopalan, venkatraman; Greenblatt, Martha, submitted, Inorganic Chemistry (2015).


Self-propelled micromotors which decompose dissolved fuel molecules to generate motion are an important class of active matter. One critical challenge is in directing the motion of such micromotors. The major barrier is Brownian motion. Brownian rotations randomize particle orientations, leading to long-time isotropic enhanced diffusion. Current strategies for directing catalytic motors include external magnetic fields, gravitational fields and electrophoretic traps. However, these strategies either lack autonomy (external fields and traps) or only constrain along 1-D (gravity). The IRG team has now demonstrated the directed motion of catalytic motors moving in close proximity to solid surfaces through active quenching of their Brownian rotation, as shown in Figure 2.1. Catalytic Janus particles in proximity to a surface undergo constrained in-plane swimming along the wall. This prolonged directed transport is not dependent on any external fields or potentials and continues for distance much longer than previously reported. The ability to steer Janus motor particles unidirectionally along complicated trajectories by simply following an edge or groove opens the door for many transport and separation tasks such as substrate-directed, flow-free microfluidics. Feature-directed steering combined with chemotaxis-directed translation could provide an ideal ‘explorer particle’ for oil or mineral exploration tasks, and more generally provides a means to guide the assembly of active colloids. One further possibility, opened up by understanding the mechanism, is that “geometric tracks” are not always needed; rather, “chemical tracks” might be sufficient to guide particles along pre-determined paths.

Such boundary walls can also conspire to produce a dead-end channel, as shown in Figure 2.2. Such dead ends are ubiquitous in nature, especially in geological and biological systems that are subject to frequent disruptions. Materials are often trapped within such pores, since fluid flows is not possible through conventional pressure-driven mechanisms. We have shown that chemically-driven convective flows leading to transport in and out of dead-end pores can occur, by the phenomenon of “transient diffusioösmosis”. Flows can reach 50 μm/s and extract otherwise-trapped materials. The IRG’s results illustrate that chemical energy in the form of a transient salt gradient can be transduced into mechanical motion, with...
the pore wall acting as the pump. This phenomena may underlie observed transport in many geological and biological systems involving tight or dead-end micro and nano-channels.

The IRG team now aims to create new porosity within rocks and minerals from which we might extract material using the flow techniques described above. One such technique is pseudomorphic mineral replacement reactions. pMRRs involve one mineral phase replacing another while preserving the original mineral’s size and texture. It is unclear precisely how replacement occurs on the molecular scale and what role is played by dissolved ion transport. We have developed a new quantitative framework to explain the pseudomorphic replacement of KBr crystal in a saturated KCl solution through a combination of microscopic, spectroscopic, and modeling techniques. Our observations reveal that pMRR is transport-controlled for this system, and that convective fluid flows caused by diffusioosmosis play a key role in ion transport across the reaction-induced pores in the product phase. These findings have important implications for understanding how pores might be created in natural minerals, which could then be exploited in industrial processes.

Turning from ion gradients to enzyme substrate gradients, the IRG continues to investigate the chemotactic separation of enzymes. We have now demonstrated a technique for the spontaneous sorting of enzymes that is based on substrate concentration-dependent diffusivity of active enzyme molecules and their chemotactic response towards imposed substrate gradients. This separation is observed within a two-inlet, five-outlet microfluidic network, designed to allow mixtures of active (ones that catalyze substrate turnover) and inactive (ones that do not catalyze substrate turnover) enzymes, labeled with different fluorophores, to flow through one of the inlets. Substrate solution was introduced through the other inlet of the device at the same flow rate. The steady-state concentration profiles of the enzymes were obtained at specific positions within the outlets of the microchannel using fluorescence microscopy. In the presence of a substrate concentration gradient, active enzyme molecules migrated preferentially toward the substrate channel. The excess migration of the active enzyme molecules was quantified in terms of an enrichment coefficient. Unlike other label-free techniques, chemotactic separation does not depend on physical properties, such as molecular size and surface charge. To validate our experimental observations, we estimated theoretical separation efficiencies for the given pairs of enzymes using multiphysics simulations. In principle, the same technique can be used to separate other active catalysts from their less active or inactive counterparts in presence of their respective substrates and should therefore find wide applicability.

In addition to the catalytic Janus particles described earlier, the IRG also continues to make important discoveries in the motion of rod-like catalytically powered swimmers, in particular
phenomena of collective assembly. The elucidation of the pairwise interactions of individual swimmers holds the key to better understanding the collective behavior of assemblies of catalytically powered colloidal objects in dynamic structures far from equilibrium, so-called “active matter.” Towards this end, the IRG studied catalytically propelled bimetallic microrods, and found that electrostatic forces drive their assembly into staggered doublets and triplets, which have different modes of motion than isolated micromotors. More recently we have fabricated and studied tri-segmented rods (e.g., Au-Ru-Au and Ru-Au-Ru), which individually do not propel in fluids because of their symmetric catalytic structure. However, these rods do catalytically pump fluids and are mimetic of microbial head-actuated “pullers” such as C. reinhardtii, or “pushers” such as E. coli, which swim by driving fluid away from their flagellar tails. The powered assembly of pushers and pullers has been modeled by several theoretical groups and recently reported in an experimental study by Shelley, et al. The focus of our work has been to measure and model the pairwise forces driving these assembly processes.

Figure 2.4: The direction of propulsion of metallic nano rods is dominated by the relative densities of the two constituent metals, not the degree of concavity/convexity of the rods ends.

Figure 2.3 shows preliminary experimental and modeling results of rod-rod pairwise interactions. We find for example that pushers at distances less than one body length experience an attractive pressure force that draws rods together with all three segments aligned. This configuration is never observed with pullers, which have an outward pressure force. The association of rods with staggered stripes (pushers) or single segment overlap (pullers) represents a balance of pressure and electrostatic forces that are generated catalytically. Experiments with polystyrene tracer particles and pushers/pullers allow us to estimate the distance dependence of both viscous forces and more long-range electrostatic forces in this system. To study the scaling of catalytic motors into the regime of tens of nanometers (where there are some conflicting results from other experimental groups) we will design nanoscale bimetallic motors that contain magnetic segments, in order to freeze rotational diffusion so that catalytic axial propulsion can be studied directly.

Figure 2.5: Rotation of microparticles and cells by an oscillating acoustically driven bubble. CW rotation of (a) doublet and (b) triplet. (c) CCW motion of HeLa cell. (d) Rotational speed $\omega$ versus driving voltage $V_{PP}$ of a HeLa cell driven by a bubble at constant excitation frequency, varying as $V_{PP}^2$. (e) Rotational angle as a function of time for a HeLa cell. Scale bar is 10 $\mu$m.
Acoustic Propulsion of Motors: The IRG discovered three years ago that metallic nanomotors could be propelled autonomously in fluids at speeds up to 200 body lengths/second by low-power ultrasound in the MHz regime. This fuel-free propulsion is interesting because ultrasound is biocompatible, and in subsequent research we and others have studied the propulsion of these motors in live cells. The propulsion mechanism was not well understood, but last year a theoretical paper by Lauga explained many of the observations on the basis of an acoustic streaming model. To test this model, we have studied axial propulsion and related effects (e.g. self-organization of rods into spinning chains) as a function of the shape, size, and composition of the motor. While we find a quadratic power dependence of axial speed, as predicted in the model, we also find behaviors that are unanticipated. Most notably, we find that the composition of bimetallic rod motors is a strong determinant of the direction of motion, with the lighter end always leading (Figure 2.4). This is an interesting finding because it suggests that new effects such as rheotaxis (autonomous propulsion directed up- or downstream in a flow) might be achievable with acoustic motors. We are currently performing experiments with acoustic propulsion of lithographically patterned motors to understand scaling and shape effects, and are working with collaborators Hoyos, Cochran, Trolier-McKinstry, and Huang on transducer design for acoustic motors that can be propelled and controlled at mm-cm distances.

Acoustically powered motility can also be used for the precise rotational manipulation of single cells or organisms, a capability that would prove invaluable for many applications in biology, chemistry, physics, and medicine. The IRG team has developed an acoustic-based, on-chip manipulation method that can rotate single microparticles, cells, and organisms, as shown in Figure 2.5. To achieve this, we trapped microbubbles within predefined sidewall microcavities inside a microchannel. In an acoustic field, trapped microbubbles are driven into oscillatory motion generating steady microvortices which were then utilized to precisely rotate colloids, cells and entire organisms (i.e., *Caenorhabditis elegans*). We have demonstrated the capability of our method by analyzing reproductive system pathologies and nervous system morphology in *Caenorhabditis elegans*. Using our device, we revealed the underlying abnormal cell fusion causing defective vulval morphology in mutant worms. Our acoustofluidic rotational manipulation technique is easy to use, compact, and biocompatible, permitting rotation regardless of the optical, magnetic or the electrical properties of the sample under investigation.

For application, cost is often a driving concern. To this end, the IRG team has demonstrated low-cost acoustic tweezers that can be used in disposable devices, as shown in Figure 2.6. Rather than forming an acoustic resonance, we locally transmitted standing surface acoustic waves into a removable, independent polydimethylsiloxane (PDMS)-glass hybridized microfluidic superstrate device for micromanipulation. By configuring and regulating the displacement nodes on a piezoelectric substrate, cells and particles were effectively patterned and transported into said superstrate, accordingly. With the label-free and contactless nature of acoustic waves, this technology could offer a simple, accurate, low-cost,
biocompatible, and disposable method for applications in the fields of point-of-care diagnostics and fundamental biomedical studies.

Acoustic fields also provide one compelling venue for generating periodic potentials in which powered micro swimmers can move, with intriguing results along the lines of those predicted by the IRG theory team in Figure 2.7. Self-motile micro/nano-particles express dynamical chirality, i.e. that which originates in motion, not structure. We have predicted how dynamically chiral objects, with overdamped dynamics in a soft periodic two-dimensional potential, can display not only separation into well-defined dynamical subclasses defined by motility characteristics, but also the ability to be steered to arbitrary locations in the plane by simply changing the amplitude of the external potential. Orientational and translational diffusion produce new types of drift absent in the noise-free case. As practical implementation seems feasible with acoustic or optical fields, these phenomena can be useful for laboratory micro-scale manipulations, possibly including reconfigurable microfluidic circuits with complex networks of unidirectional channels. In additional theory advances, we have developed a elegant model of electrocatalytic propulsion within a self-consistent non-local feedback framework, provided an analytical treatment of spheroidal electrocatalytic swimmers, and have extended our kinematic matrix formalism to encompass additional memory effects, as a first step to describing hysteretic motility, which we anticipate will be a rich source of collective phenomena in active systems.

The IRG team has also demonstrated facile in situ fabrication and acoustic actuation of microrotors, as shown in Figure 2.8. A polymeric microrotor with predefined “beak” structures is fabricated by applying a patterned UV light through a photocrosslinkable polyethylene glycol (PEG) solution and polymerizing inside a microchannel while in-place around a polydimethylsiloxane (PDMS) axle. Piezoelectric transducers (PZTs) generate tunable acoustic waves which actuate the microrotors by oscillating the beak structures and thus generating acoustic streaming. The thrust generated by the acoustic streaming flows

Figure 2.7: Drift-phase behavior for a counterclockwise chiral swimmer with and without orientational and translational diffusion, showing how variation in the orbital radius of the swimmer (\(\beta\)) and the strength of a symmetry-lowering periodic external potential (\(\alpha\)) cause qualitative changes in the swimmer’s motion. Simply changing the strength of the periodic potential can induce a swimmer to drift to any desired location in the plane.
rotates the microrotors with a tunable rotational rate controlled by the peak-to-peak voltage applied to the transducer. A 6-armed microrotor can exceed 1200 RMP. This technique is an integration of single-step microfabrication, instant assembly around the PDMS axle, and easy actuation. These acoustic driven microrotors can be used in various applications including micropumps, micromixers, and microgears.

Moving forward, we hope to achieve a hierarchical understanding of the 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.

Figure 2.8: (a)-(f) Image series for an acoustically actuated 6-arm microrotor, showing a full rotation across 6 frames. (g) RPM versus peak-to-peak voltage for a 6-arm microrotor, showing a linear increase of the angular speed with the applied voltage amplitude, above a small offset voltage (~20–30V) necessary to initiate motion.
IRG 3: HIGH-PRESSURE ENABLED ELECTRONIC METALATTICES
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IRG3 has made significant progress in synthesizing and charactering metalattices, which we define as artificial 3D solids that are periodic on a scale of 1–60 nm. An important difference between metalattices and quantum dot superlattices or porous semiconductors is that an ordered, highly interconnected surface or interface interweaves the structure. Depending on the the detailed structure, the metalattice could be notionally subdivided into “meta-atoms” (e.g. more capacious regions) linked by “meta-bonds” (e.g. thin channels that interconnect meta-atoms). Metalattices provide new platforms for the study of semiconductors stressed to allow for tuning of bandgap by as much as ~2x, metal-insulator transitions, artificial magnetic systems, and novel optical response in semiconductors. Ultimately, many other physical regimes could become available, such as thermoelectric systems with tuned lattice thermal/electrical conductivity, and possibly long-wavelength charge ordering. IRG3 synthesizes metalattices using high pressure confined chemical vapor deposition (HPcCVD) of semiconductors and metals into nanotemplates with appropriate periodicity. Accomplishments for the reporting period include synthesis of metalattices with smaller periodicities, new compositions, and new symmetries, removal of templates from these metalattices, characterization of the electrical transport and photoluminesence properties of elemental semiconductor metalattices, advances in the theory of the thermal transport and thermoelectric properties of metalattices and identification of new ultra-low frequency Raman modes of vibration in them. This latter observation may be the first experimentally observed manifestation of the nanoscale periodicity of metalattices. Metalattices are also emerging as a versatile platform to understand semiconductor luminescence properties because such properties can be investigated for different materials that are precisely structured with the same symmetry as the length scale is changed from the quantum size regime to tens of nm and the surface chemistry is varied. The ability of HPcCVD to fill nanotemplates void-free with materials has also been modeled and investigated experimentally.

Metalattice Templates with Smaller Periodicities and New Symmetries: Using an amino acid-catalyzed silica colloid synthesis, colloidal crystal templates with a range of sphere sizes from 14 nm to 250 nm have been grown. High quality colloidal crystal films with lateral dimensions up to at least 1 cm² have been grown by in ovens with carefully controlled temperature and humidity. The IRG is investigating the replication of colloidal crystals with several types of flexible polymers and have demonstrated the ability to reduce the scale of the lattice while maintaining order. This allows us to potentially use larger, more
synthetically facile colloidal crystal templates to access three dimensionally ordered templates for metalattice synthesis with unit cell dimensions in the range of 2 to 10 nm, a size range for which such templates are in general difficult to find. Using positron annihilation spectroscopy (PALS), we have found that silica spheres annealed at 600 °C exhibit undesired nanopores within their interior structure whereas this porosity is annealed out at 800 °C.

To obtain more complex template geometries to allow for metalattices with different symmetries, connectivities, and periodicities and thus properties after void-free filling with semiconductor, we have also grown binary silica colloidal crystal films (Figure 3.1 top). Producing large phase-pure crystals remains a challenge for future work. We are addressing this challenge by constructing phase maps to determine ideal growth conditions for crystal phases of interest. During these studies, we discovered that small silica colloids (~100 nm diameter or less) adjust their shape during crystal film growth (Figure 3.1 bottom), transitioning from an initially spherical shape to polyhedral shapes that are determined by lattice packing. This shape ripening depends upon the local colloidal packing environment and deposition conditions. So far, shapes that have 2-D cross sections that are triangular (likely a 3D tetrahedron), square (likely a 3D cube; fig. 1 bottom), hexagonal, octahedral, and tear-drop shaped have been observed. Understanding the mechanism behind this behavior could provide valuable knowledge about the stability and packing geometry of evaporation-driven colloidal crystal assembly.

Metalattice Synthesis: The ability to systematically vary periodicity and also modify properties via appropriate modification of surface chemistry and/or additional deposition steps in metalattices is valuable to understanding their thermal, electronic, optical, and magnetic properties. With these goals in mind we have synthesized silicon and germanium (Figure 3.2a) metalattices from templates consisting of silica spheres as small as 14 nm in diameter and for the first time have removed the sphere template (Figure 3.2b,c). This latter step represented a challenge because nanostructures with periodicities in this size range often collapse upon template removal. Intrinsic, p-type, and n-type doped silicon metalattices have been synthesized from appropriate precursors. 14 nm metalattices have ~3 nm meta-atoms approaching the size regime for quantum confinement in silicon. Using atomic layer deposition (ALD), alumina and hafnia have been deposited inside silicon metalattices that first had the template removed, allowing for investigation of the impact of surface passivation on metalattice
photoluminescence. We have also deposited germanium inside such "empty" silicon metalattices. We plan to investigate the synthesis of magnetic silicide metalattices via a similar approach.

Platinum and nickel metalattices were synthesized as a first step towards a variety of metal metalattices that could have interesting magnetic and superconducting properties. We have deposited silver as well into sphere templates, but must modify the template surface chemistry to allow for void-free deposition. The IRG team is also tuning precursor chemistry to make well-developed metalattices of materials such as ZnSe and other chalcogenide/magnetic semiconductors. We have found that zeolites, ordinarily extremely beam sensitive, become nearly indefinitely stable to electron beam irradiation at 200 keV upon infiltration, suggesting they have been stabilized by it. Chemical mapping of Ge via TEM in zeolite infiltrated metalattices further confirms infiltration has occurred. We have also investigated the crystallization of metalattices composed of amorphous silicon; in contrast to the lowering of the crystallization temperature observed in silica fiber templates, the nanostructure of the metalattice raises the crystallization temperature by as much as 75 degrees.

**Kinetics of Silane Decomposition in HPcCVD:** An experimental and theory study of the kinetics of the thermal pyrolysis of silane at HPcCVD pressures revealed that the growth rate is first order in silane concentration with an activation energy of 53.7 kcal/mole. This activation energy is in the range of those expected for hydrogen desorption reactions at a crystalline silicon surface, suggesting that this process is the rate limiting step. These observations were corroborated by reactive molecular dynamics simulations, which also show that (as is experimentally observed) heterogeneous reaction is expected to dominate over homogeneous reaction in HPcCVD. These insights may suggest means to modify surface chemistry to increase reaction rates or lower reaction temperatures to facilitate use of "soft" metalattice templates.

**Positron Annihilation Spectroscopy (PALS) of Metalattices:** To quantitatively assess whether metalattice templates are truly filled (TEM and SEM are only qualitative, at least for larger periodicity metalattices) without voids to give geometrically well developed metalattices, the IRG has begun PALS investigations. After investigating the nanovoids present in the unfilled silica sphere templates, we can conclude that annealed crystalline silicon metalattices formed from 30 nm sphere templates are truly void free, as there is no PALS signal from them. We next plan to use PALS to investigate the porosity of semiconductor and metal metalattices synthesized using other templates, including aerogels, zeolites, Vycor glass, and metal-organic frameworks.

**Metalattice Photoluminesence:** Si and Ge metalattices both display a broad visible luminescence band, as is observed in other nano-structured silicon systems such as porous Si and colloidal Si nanocrystals. Our investigations are giving insight into the role of quantum confinement and surface state trapping on metalattice electronic properties. In particular, the ability to systematically change the (precisely controlled) metalattice dimensions and symmetry as well as the type of infiltrated semiconductor and surface passivation makes metalattices an excellent platform for understanding.
luminescence in porous semiconductors more generally. We find negligible photoluminescence in these structures until after annealing at high temperature to crystallize them. The strikingly similar shapes of the silicon and germanium metalattice photoluminescence spectra (Figure 3.3) suggest that the semiconductor itself is not the source of the luminescence. Rather, it appears that the semiconductor strongly absorbs incident light, resulting in energetic free carriers that quickly reach an interface and become trapped. Radiative recombination within this inhomogeneously broadened distribution of interface sites is currently thought to be the source of light emission. Future plans include investigations of a wider range of metalattice sizes and additional measurements such as ultrafast transient absorption to monitor carrier relaxation and trapping kinetics. 14 nm metalattices display a much more complex photoluminescence spectrum that may be associated with quantum confinement. First-principles and empirical tight-bonding calculations of the electronic structure and optical response of Si and Ge metalattices, with particular attention paid to surface and interface effects, are underway to elucidate the origins of these phenomena.

Ultra-Low Frequency Raman Spectroscopy of Silicon Metalattices: In general, ultralow frequency Raman is useful in probing the vibrations of entire nanostructures,15-17 In particular, periodic nanostructures such as semiconductor superlattices may exhibit ultra-low frequency Raman modes associated with their periodicity.17 We find a series of peaks in the low frequency Raman spectrum of a metalattice synthesized from a 30 nm silica sphere template (Fig. 4). These peaks may similarly be associated with the periodicity of the metalattice; a 14 nm metalattice, for example, shows a different pattern of low frequency peaks. No such peaks were found in the Raman spectrum of a silica sphere template, suggesting that they are not associated with Lamb modes of oscillation15 of silica spheres.16 The low frequency upturn upon which the peaks are superimposed may be associated with intervalley carrier scattering.18 We plan further investigations into the low frequency Raman spectra of metalattices with different sizes and periodicities, with and without their templates intact to better understand the observed spectra. These spectra may be the first experimental manifestation of the 3-dimensional periodicity of metalattices. Simulations of lattice dynamics in these metalattice systems are being pursued in concert with these experimental measurements.

Transport Measurements: Using a simple approach to Van der Pauw measurements with evaporated contacts we find that phosphorus-doped n-type silicon metalattices from 30 nm sphere templates have a greater resistivity (~40 Ω·cm at 300 K) than n-type silicon films (~0.4 Ω·cm) deposited in the same HPeCVD reactor. A plot of resistivity vs. T14 reveals a straight line suggestive of variable range hopping. We are plan to synthesize metalattices with thicker meta-bonds to increase the electrical conductivity. We are now developing a lithography-based process to fabricate four-terminal transport devices, Hall bars, and devices for measurement of thermoelectric power. Bulk thermal transport measurements vs. temperature via the 3ω and time-domain thermoreflectance19

Figure 3.4. Ultra-low frequency anti-Stokes Raman spectrum of silicon metalattice synthesized via infiltration into a 30 nm silica sphere template. The template was not removed. A series of low frequency peaks are observed superimposed on a low frequency upturn on both the Stokes and Anti-Stokes side of the excitation line. These peaks may be associated with collective vibrations of the metalattice. The low frequency upturn upon which the peaks rest may be associated with inter-valley scattering of carriers. A Si wafer reference spectrum with a Brillouin peak is shown for comparison.
methods are planned for the coming year to investigate the impact of metalattice periodicity on thermal conductivity. Measurements of the nanoscale heat transport mechanisms in metalattices via high harmonically generated ultrafast extreme UV techniques\textsuperscript{20,21} are planned for the coming year. Along these lines, the IRG team has developed a novel coherent diffraction imaging technique based on ptychography that enables simultaneous full-field imaging of multiple, spatially separate, sample locations. This approach enables spatially resolved polarization spectroscopy from a single ptychography scan, as well as allowing a larger field of view to be imaged without loss in spatial resolution and will be useful in the characterization of metalattice samples.

The IRG team will also pursue electrical transport measurements on other metalattices, in particular silver-germanium devices. The interface between silver and germanium can exhibit interface superconductivity.\textsuperscript{22} The high surface area of the infiltrated metalattices will allow for previously inaccessible bulk-type measurements of this interface superconductor. Additionally, the unique geometry should lead to novel effects related to the dynamics of Abrikosov vortices in these devices.

**Molecular Dynamics Simulation of Heat Transport in Silicon Metalattices:** Modeling of heat transport in metalattices reveals the physics of phonon scattering in the regime where the length scales of the lattice are comparable with the mean free paths of the heat-carrying phonons. To model heat transport, we employed a modified Stillinger–Weber potential whose parameters have been fitted against first-principles density-functional theory data using a force-matching method. Green–Kubo autocorrelation calculations were used to compare the various factors affecting the lattice thermal conductivity in Si metalattices (Figure 3.5a). While scattering by isotopic impurities causes a significant lowering in the lattice thermal conductivity, the insertion of 1–10 nm voids led to a much larger decrease in thermal conductivity. We found that passivation of the void surfaces by oxygen provides an appreciable reduction in the lattice thermal conductivity, whereas passivation by hydrogen does not lower heat conductivity significantly. We observed that isotopic mass disorder after the introduction of nanopores provided the largest decrease in heat transport down to 0.25–1 W/mK. We finally examined how the heat conductivity of Si metalattices varies with the volume fraction of the nanopores at both the atomistic and continuum levels. These calculations revealed that the dependence of thermal conductivity on the volume fraction of the nanopores differs markedly from the behavior expected from continuum theories due to the influence of interface scattering (Figure 3.5b). To further examine these results, we are now performing a frequency-resolved analysis of the phonon mean.

Figure 3.5: (a) Molecular dynamics predictions for the lattice thermal conductivity of bulk and nanoporous silicon in the temperature range of 300–1000 K taking into account isotope effects, the size and arrangement of the nanosized voids, and surface passivation by hydrogen or oxygen. (b) Comparison of continuum and molecular dynamics predictions for the lattice thermal conductivity of Si metalattices; phonon scattering at the surface of the nanopores in molecular dynamics simulation leads to much steeper decrease in the thermal conductivity than expected from continuum calculations.
free paths in bulk and nanoporous Si using spectral Green–Kubo techniques. This analysis will explain how short- and long-wavelength phonons are affected by the presence of nanopores to provide a predictive understanding of frequency-dependent scattering processes in metalattices to help design nanostructures with low thermal conductivity.
References


IRG4: MULTICOMPONENT ASSEMBLIES FOR COLLECTIVE FUNCTION

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In its first year, the new IRG4 effort has forged strong working relationships between the students in different departments and has acquired exciting new results in each of the four main project areas: (P1) Collective function in metal-insulator transition nanoparticle arrays; (P2) Emergent optical properties of nanocylinder assemblies; (P3) Particle assemblies with tunable disorder for linear and nonlinear photonics; and (P4) Illumination-directed assembly of photoresponsive semiconducting particles.

P1. Collective function in insulator-to-metal transition (IMT) nanoparticle arrays:
This effort aims to produce coupled VO$_2$ nanostructures by directed assembly of solution-synthesized nanoparticles. In Year 1, we employed top-down fabricated VO$_2$ to study phase behavior and electrical processes while we worked to develop synthetic and assembly strategies.

Quantitative nanoscale impedance mapping of the spatially inhomogeneous IMT in VO$_2$ has been performed with a lateral resolution of 50 nm through near-field scanning microwave microscopy (SMM). SMM spatially resolves electronic properties of the phase coexistence in an unstrained VO$_2$ film during the electrically as well as thermally induced IMT. A quantitative impedance map of both the electrically driven filamentary conduction and the thermally induced bulk transition was measured and also modeled as a 2-D heterogeneous resistive network where the distribution function of the IMT temperature across the sample is captured. Applying the resistive network model in an electrically induced IMT, we reproduced the filamentary nature of electronically induced IMT, which elucidates a cascading avalanche effect triggered by the local electric field across nanoscale insulating and metallic domains.

We also developed a Ginzburg-Landau (GL) free energy to describe the thermodynamics of VO$_2$. This model incorporates the electron degrees of freedom in addition to order parameters characterizing the structural differences between the rutile and monoclinic phases. The predict-

![Figure 4.1. (left) Schematic of the near-field scanning microwave microscopy characterization of VO$_2$ IMT thin films (ACS Nano 2015, 9, 2009-2017). (center, right) Domain structure of [110]-oriented VO$_2$ thin film obtained from a preliminary phase-field simulation with a mismatch strain $\varepsilon_S = 0.003$. (center) $T = 330$ K and (right) $T = 350$ K. At 330 K, the simulation predicted a domain structure with order parameters $\mu = 0$ and finite $\eta$, indicating a “monoclinic metal” (indicated as MM). We start to see the appearance of the high-temperature rutile (R) phase at 350 K and thus the phase coexistence of the R phase and a low temperature monoclinic (M2) phase at 350 K.](image-url)
ed temperature-stress phase diagram from the free energy model agrees well with the experimentally measured diagram. The IRG is currently studying the domain structure evolution as the crystal goes through the metal-insulator transition. The center and right panels of Figure 4.1 show domain patterns obtained in a VO₂ film constrained by a substrate from phase-field simulations at 330 K and 350 K. We will next perform phase-field simulations of the domain evolution in VO₂ oscillators under an electrical current as well as the phase stability and domain structures in VO₂ nanoparticles in coordination with the experimental work.

In synthetic work, we have achieved scalable, high yield hydrothermal synthesis of VO₂(M1) nanoparticles from solution. Particles were characterized by electron microscopy, XRD, Raman, and DSC. In contrast to traditionally grown epitaxial VO₂ films (discussed above), solution-synthesized VO₂ nanoparticles can be deposited onto arbitrary substrates. Synthesis conditions could be systematically tuned to produce wires, cubes, and star-shaped particles (Figure 4.2a shows wires). The IRG is now investigating the reaction mechanism and expanding our reaction methodology to other metal oxide systems, including NbO₂ and Al₂O₃ (of interest for IMT and optical applications, respectively). The monodispersity in size and shape for individual VO₂ particles approaches what is needed for assembly, however nanoparticle clusters are not uncommon and respond preferentially to applied fields. Efforts to minimize clustering by adjustments in the wire synthesis are ongoing, but even assembly of bundled clusters is of interest, as they are expected to exhibit switching and hence could be useful from a device perspective. Assembly is shown in Figure 4.2b,c. Preliminary measurements of single VO₂ wire electrical response suggest sample oxidation during the fabrication process. To stabilize the VO₂ (M1) phase against post-synthesis oxidation, and to prevent particle self-association, the IRG team is identifying appropriate surface ligands.

**P2. Emergent optical properties of nanocylinder assemblies:**

The IRG team is taking advantage of dielectrophoresis and e-field induced dipolar interactions between assembled particles to generate ordered two-dimensional (2D) lattices of silica coated solid and segmented Au nanowires (Figure 4.3a-d, Langmuir 2015). These lattices are field-responsive and can be reconfigured in real time by altering the applied field. Dielectrophoretic forces from the ac field concentrate wires between the electrodes, with their long axis aligned parallel to the field lines. After reaching a sufficient particle density, field-induced dipolar interactions result in the assembly of dense 2D lattices that span the electrodes, a distance of at least ten wire lengths. The ends of neighboring Au wires or segments overlap a fraction of their length to form lattice structures with a “running bond” brickwork-like pattern. The observed lattice structures are tunable in three ways: (1) particle segmentation pattern, which fixes lattice periodicity for a given field condition; (2) ac frequency, which varies lattice periodicity in real time; and (3) switching the field on/off, which converts between lattice and smectic particle organizations. Electric field simulations were performed to understand how the observed lattice
periodicity depends on the assembly conditions and particle segmentation. Directed self-assembly of well-ordered 2D metallic nanowire lattices that can be designed by Au striping pattern and reconfigured by changes in field conditions could enable new types of switchable optical or electronic devices. We are currently working to generate reconfigurable infrared polarizers based on reconfiguration of these nanowire lattices (Fig 4.3e-g). Simulations indicate excellent discrimination between polarized light aligned parallel vs. perpendicular to the nanowire long axes in the lattices, and preliminary experimental results show a similar trend. Work is underway to alter polarization response in real time by reconfiguring the orientation of the entire lattice using quadropolar electrode geometries.

In the absence of an applied field, particle assembly onto patterned surface features generally requires either chemical binding (e.g., H-bonding, hydrophobic interactions, or biorecognition) or electrostatic interactions between chemical groups on the particle surface and the surface features. This often requires chemical functionalization or one or both surfaces and can pose additional limitations both on the assembly process and on the interfacial spacing and structure between the particles and the surface. Thus the IRG is exploring the potential of patterned van der Waals’ interactions for directing self-assembly. Experimental results indicate that gold nanowires preferentially assemble onto gold patterns on a silica substrate. This effect persists when both the wires and the entire substrate are coated with a thin layer of silica to avoid any variation in electrostatic interactions across the patterned substrate. We are simulating this assembly using a Monte Carlo approach, with 3 types of wire-substrate interactions: vdw interactions between the pad and the nanowires $E_{vdW,\text{pad-wire}}$, vdw interactions between the nanowires $E_{vdW,\text{wire-wire}}$, and electrostatic (ES) interactions between the nanowires $E_{ES,\text{wire-wire}}$. The electrostatic interaction between the nanowires and the substrate is assumed to be uniform, as is the gravitational force, so these can be neglected. Therefore, we define the total energy as: $E_{tot} = E_{vdW,\text{pad-wire}} + E_{vdW,\text{wire-wire}} + E_{ES,\text{wire-wire}}$. Our model shows qualitatively similar behavior to the

![Figure 4.3](image-url)

**Figure 4.3.** Nanowire lattice assemblies. (a) Coplanar electrode setup, showing stem/bulb (S/B) geometry and transmitted optical image of electrode gap. TEM images of particles (b) 2.5Au and (c) 2.5Au-1E nanowires. (d) Reflectance optical image of assembly for 2.5Au-1E nanowires. (Langmuir 2015, 31, 5779). (e-g) Simulation of polarization dependent transmission of gold nanowire lattices. (e) Unit cell used in the simulation with polarization of incidence light. (f) Simulated transmittance of linearly polarized light through a single layer of aligned nanowires in water (n=1.3). $D=170\,\text{nm}$ and $L=3\,\mu\text{m}$, (g) Experimental transmittance of polarized light for 170 nm Au wires assembled in lattice.
experimental system both in terms of the nanowires concentrating on the gold substrate features and also in their orientation on the features. We are comparing the number of wires/area and their average orientation angle and working to further optimize the model, which already comes close to describing several experimental scenarios with different wire length and substrate feature dimensions (Figure 4.4).

One major functional target for these assemblies is “wrapped” metasurfaces to control electromagnetic field distributions. Along these lines, the IRG team has demonstrated ultra-lightweight metasurfaces, comprised of subwavelength electric and magnetic resonator arrays capable of fully restoring the intrinsic properties of real-world radiators in a multi-radiator environment (Figure 4.5, top). We are working to translate this concept from radio to optical wavelengths utilizing electric field-directed nanowire assembly and patterned substrate topography as nucleation sites. Simulations suggest nanowires organized around a dielectric post can accomplish a near-zero scattering signature, cloaking the post (Figure 4.5, middle). To that end, we are developing new methods to vertically assemble cylindrical particles around a central feature, such as a photoresist or amorphous silicon post. AC electric field is applied vertically and leads to vertical orientation of wires, with relatively evenly-spaced particles around the posts where the field gradient is steepest (Fig 4.5, bottom). In the coming year, the IRG team will evaluate the impact of various classes of assembly defects on expected performance (by simulation) and will shift to smaller feature size in the experimental assemblies to better match simulation conditions. As the particle diameter decreases, the operating wavelengths of these devices will shift to shorter wavelengths. Several exciting optical devices can be generated from these general types of assembly geometries, including not only metasurfaces but also emitters of illumination with orbital angular momentum. All these approaches will emphasize reconfigurability to alter the optical response by changing the particle assemblies with applied field conditions.

Figure 4.4. Simulations for vdW-driven assembly of gold wires onto gold features on a silica substrate. (a) Images for wire position after two initial simulation conditions. (b, d) Potential energy of the system during the simulation process, showing that perfect and random initial scenarios approach each other with increasing steps. (c, e) Wire orientation on the gold features showing that experimental orientations are intermediate between simulations from the random and perfect starting conditions. Panels (b, d) correspond to (a), and (d,e) to a system with wire length 2.4 μm and gold stripe width 4.3 μm.
**P3. Particle assemblies with tunable disorder for linear and nonlinear photonics:**

The IRG team is investigating operation of single mode tunable semiconductor micro-ring lasers near exceptional points for use as ultra-sensitive nanoparticle detectors. An optical platform comprising two identical coupled micro-rings is a simple yet efficient means of observing exceptional point dynamics. Keeping one ring in the dark while shining pump light over its counterpart creates a balanced gain-loss profile. By varying the gain/loss contrast, one can reach the exceptional point where the two split resonance lines just fuse together. Upon a slight perturbation of this system, the degeneracy in the eigenvalues is lifted with a splitting proportional to the square root of the perturbation. We are using particle assembly to provide this perturbation, with real-time reconfigurability.

As a first step towards the IRG’s goals in disordered photonics, we have demonstrated random lasing in particle-dense suspensions of silica beads surrounded by a matrix of ethanol that contains a laser dye. We have also demonstrated real-time control over silica particle packing density by changing applied field conditions. The team has nearly completed construction of an experimental setup that will enable simultaneous electric-field directed particle assembly, imaging, and collection of either lasing or scattering spectra, and hope to soon control lasing onset and properties while following particle position within the assemblies.

**P4. Illumination-directed assembly of photoresponsive semiconducting particles:**

Illumination-controlled assembly of amorphous silicon (aSi) particles has been achieved with discs and cubes produced by top-down fabrication as well as in mixed-particle assemblies where only one type of particle responds to light, in which the photoactive particles are switched between positive and negative dielectrophoresis. Figure 4.7 shows this effect for aSi cubes: under illumination they exhibit positive DEP, migrating to regions of highest field intensity (stem regions of the coplanar electrodes) while under low-light conditions they move to regions of lower electric field (bulbs). We have evaluated several other particle types for illumination-responsive assembly and have found that for some particles, surface properties of the particles can dominate the assembly behavior such that negative DEP is not achieved in low-light conditions. This is consistent with the well-known positive DEP behavior of some dielectric particles (e.g., polystyrene) in DI water. The IRG plans systematic studies of the assembly behavior (e.g. crossover frequency between positive and negative DEP) as a function of surface charge.

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**Figure 4.5. (top)** Schematic and photograph for metasurface coatings on macroscopic antennae. From Werner & coworkers, *Adv. Funct. Mater.* 2015, 25, 4708. *(middle)* Schematic and simulation for the impact of a ring of gold nanowires around a 0.5 μm silicon post on the field distribution at 3.64 μm. When wires are present *(right-hand panel)*, the post is cloaked. *(bottom panels)* Assembly setup and image of gold nanowires assembled around photoresist posts, viewed from top.
(measured as zeta potential). Surface functionalization with organic or inorganic coatings will alter the interfacial properties as needed. As we develop a library of illumination-responsive particles, we will incorporate them into the assemblies described above to further control both the assembly process and the properties of the resulting devices.

The IRG team has also explored the possibility of local heating by focused illumination both as an assembly tool (for example, vertical wire assemblies are facilitated by the resulting fluid flow), and to learn how to minimize its effects for clean interpretation of charge carrier density effects in DEP response.

Using a thermocouple to monitor local temperature, we found that while heating could be significant upon illumination with a tightly focused (100x, 1.4 NA lens) unfiltered Hg arc lamp, no temperature rise was observed under a wide range of imaging and unfocused illumination conditions, even in the presence of light-absorbing metal particles in aqueous suspension. These findings demonstrate our ability to avoid sample heating during illumination at lower powers and to evaluate whether local heating is occurring. These factors will be important in differentiating effects of illumination on photoresponsive particles going forward.

Figure 4.6. Using directed self-assembly to tune the modes in micro-ring systems. (a) Schematic of parity-time-symmetric sensor showing impact of a particle near the ring. (b) SEM image of the Si micro-rings. (c) Strategy for placing particles on only one of the two rings using e-field directed assembly. (d) Assembly showing a large number of particles around only the lower ring.

Figure 4.7. Illumination-responsive assembly.
**Seed: Magnetic 2D materials**

Jun Zhu (lead), Vincent Crespi, Thomas Mallouk, Joshua Robinson, Mauricio Terrones; students, Simin Feng, An Nguyen, Youjian Tang, Junjie Wang, Kehao Zhang, 0 postdocs

The magnetic 2D seed project aims to discover new atomically thin magnetic materials based on transition metal dichalcogenides (TMDs) and explore electronically tunable magnetism in low dimensions. In 2014, the seed project pursued two parallel routes to synthesize magnetic 2D semiconductors. The first synthetic route seeks to dope MoS₂ using organic Mn precursors in situ during the chemical vapor deposition process of monolayer MoS₂. HRTEM studies show that up to two atomic percent of Mn can be successfully substituted into the MoS₂ lattice in samples grown on graphene substrates. On the other hand, doping Mn into MoS₂ grown on SiO₂ or sapphire substrates proves to be more difficult, where attempts to incorporate Mn in the growth appear to lead to more defective MoS₂, as suggested by electrical transport and PL measurements. The contrast highlights the critical role played by the reactivity of the substrate. The results are published in Nano Letters (2015) and provide important insights to the doping effort in TMD materials.

The second route seeks to synthesize Mn-intercalated (W, Nb)S₂ alloys using the chemical vapor transport method, with the objective of achieving a novel class of magnetic half-semiconductors that can potentially be useful in spintronic devices such as diodes and spin filters. The synthesis effort is closely coupled to and guide by first principles calculations, which have identified a group of Mn-intercalated compounds with the chemical formula of MnₓMo₁₋₂ₓTa₂ₓS₂ to be thermodynamically stable against decomposition and possess spin polarized conduction and valence bands. The synthesis of the identified compounds had been a challenge. Ongoing efforts are exploring alternative methods to adsorb/intercalate Mn to semiconducting TMDs. One such attempt employs the UV photolysis of dimanganeseedecacarbonyl, Mn₂(CO)₁₀ in the presence of electron-deficient TMDs NbS₂ and TaS₂. The goal of this study is to functionalize the basal plane surface with magnetic Mn(CO)₅ fragments via Mn-S bonding. XPS experiments showed the presence of Mn in these samples. Follow up photolysis experiments with CpMn(CO)₃ gave promising preliminary results, showing the presence of CO-containing complexes (possibly CpMn(CO)₂ or CpMn(CO), Cp = cyclopentadienyl) by infrared spectroscopy. Future experiments will characterize the electronic and magnetic properties of these surface-functionalized TMDs as a function of the surface coverage of the metal carbonyl complex. We will also perform control experiments with semiconducting MoS₂ and WS₂ to determine if only electron-deficient TMDs can undergo this kind of photochemical functionalization.

The seed team has also initiated a third thrust to explore the synthesis and properties of GaSe, a two-dimensional layered semiconductor predicted to exhibit carrier density tunable ferromagnetism in the few-layer limit. GaSe is a wide gap semiconductor with a band gap of ~3 eV in the monolayer limit. It is also easily oxidized in ambient conditions. We are working to develop methods of passivation to preserve the sample integrity, as well as methods to make electrical contacts.
**Seed: Superconductivity and Fluxon Trapping in Long Nanowires**

Moses Chan (lead), John Badding Jainendra Jain, Chao-Xing Liu; Students Jesse Bischof, Jue Jiang. Postdoc; Weiwei Zhao

The Seed team has completed an experiment showing a single superconducting flux quantum, or a fluxon, can be exploited to switch the resistance of a long nanowire between two discrete values. The wire is confined in hollow silica fiber of 150 nm diameter. The experimental geometry consists of such a 6 mm-long nanowire of superconducting Ga–In eutectic, with spontaneously formed Ga nanodroplets along the length of the nanowire. The nonzero resistance occurs when a Ga nanodroplet traps one or more superconducting fluxons, thereby driving a Josephson weak-link created by a second nearby Ga nanodroplet normal. The fluxons can be inserted or flipped by careful manipulation of the magnetic field or temperature to produce one of many metastable states of the system. These results are published in Nano Letters (15 153–158 (2015)). X-ray fluorescence measurements carried out at the Advanced Photon Source showed the suppression of phase separation seen in the Ga-In system is due to metastable states that arise upon nano-confinement. The Laue micro-diffraction measurements show that the wires are crystalline and that the crystal grains are quite large for a sample that is exactly at the eutectic point. The results of these structural studies are being prepared for publication.

We have completed a study on the physical origin and the nature of superconductivity of individual cylindrical single-crystal Bi nanowires of 20 and 32 nm in diameter. In contrast to nonsuperconducting Bi nanoribbons with flat surfaces, these nanowires show superconductivity below 1.3 K. However, their critical magnetic fields decrease with their diameter, which is the opposite of the expected behavior for thin superconducting wires. Quasiperiodic oscillations of magnetoresistance were observed in perpendicular fields but were not seen in the parallel orientation. These results can be understood by a model of surface superconductivity with an enhanced surface-to-bulk volume in small diameter wires. The superconductivity originates from the strained surface states of the nanowires due to the surface curvature-induced stress. These results are published in Nano Letters (vol. 15, 1487-1492 (2015)).

We also collaborated with Jagadeesh Moodera of MIT in the study of Quantum Anomalous Hall (QAH) effect in ferromagnetic topological insulator Vanadium doped (Bi, Sb)\textsubscript{2}Te\textsubscript{3} films. We observed a robust zero-field quantized Hall plateau accompanied by a negligible longitudinal resistance and also demonstrated dissipationless edge transport in the film and identified the physical origin of dissipative channel. These results were published in Nature Materials (14 473–477 (2015)) and Phys. Rev. Lett. (115 057206, 2015). In addition, transport measurements carried out by us together electron energy loss spectroscopy studies verified the Van Vleck nature of the long-range ferromagnetic order in the Vanadium doped (Bi, Sb)\textsubscript{2} Te\textsubscript{3} films. This result was published in Phys. Rev. Lett. (114 146802, 2015).

The QAH effect in a 4QL (Bi\textsubscript{0.29}Sb\textsubscript{0.71})\textsubscript{1.89}V\textsubscript{0.11}Te\textsubscript{3} film measured at 25mK. a. Magnetic field dependence of the longitudinal resistance $\rho_{xx}$ (red curve) and the Hall resistance $\rho_{yx}$ (blue curve). b, c. At low field $\rho_{yx}$ exhibits a value of 1.00019±0.00069$h/e^2$ and $\rho_{xx}$ is only $-0.00013±0.00007h/e^2$ (∼3.35±1.76Ω).
Seed: Single Layer Group III-Nitride Materials via Graphene Encapsulated Growth
Joan M. Redwing and Joshua A. Robinson

A new Seed effort was initiated in Fall 2015 to investigate a novel route to the synthesis of monolayer and few layer films of III-V semiconductors – graphene encapsulated growth (GEG). This process utilizes controlled intercalation and reaction of group III and V precursors within the interfacial region of quasi-free standing epitaxial graphene formed on SiC to form stable ultrathin III-V films. The investigators have used this approach to fabricate 2D bilayer GaN that exhibits a bandgap energy on the order of \(~5.7\) eV (as measured by low loss electron energy loss spectroscopy (EELS)) considerably larger than the 3.4 eV bandgap of bulk GaN. This seed project builds upon these exciting results to further develop the GEG approach for 2D GaN synthesis to produce larger area films, investigate the electrical properties of graphene/2D GaN heterostructures and extend the GEG method to demonstrate 2D InN and AlN compounds. If successful, this seed project could lay the foundation for a larger multi-investigator effort on ultrathin III-Vs – an entirely new class of 2D materials. Collaborations are beginning with a number of MRSEC faculty including Nasim Alem (ultrahigh resolution TEM/low loss EELS), Suman Datta (2D GaN band structure simulations) and Long-Qing Chen (first principles studies of interfacial energies and phonons in graphene/2D GaN heterostructures).
6. Education and Human Resources

The Center for Nanoscale Science is building upon its longstanding tradition of leadership in STEM outreach and education efforts at Penn State. Given the strong evidence of its institutional-level impact on K-12 informal education and summer undergraduate research endeavors, it is now focusing its efforts toward university-wide improvements regarding diversity, and graduate admission, professional development, and retention. 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 were created and are led by the Center itself, while others are led by partners with direct MRSEC involvement and participation.

Center Participation: The personal involvement of Center members is vital for the effective integration of research with educational content in outreach programs. It is also essential for the development of well-rounded research professionals and a cohesive community. Center faculty, students, postdoctoral scholars, researchers, and staff at Penn State are expected to contribute at least 12 hours per year to outreach activities. Additionally, many former Center members and affiliated researchers are frequent volunteers. During the past year, a new “MRSEC Outreach Team” structure has been conceived, organized, and approved for implementation in the coming year. The purpose of the team model is to better organize the education, outreach, and diversity-focused opportunities so that Center members can engage in them at a more sustained and meaningful level, with a stronger potential impact on their professional development.

Strategy: The Center strives to expand awareness of its research expertise, engage diverse audiences at multiple academic levels and points along the career path, positively impact Center members and volunteers, and further develop the quantity and quality of pipelines to underrepresented and underserved groups. Target audiences include undergraduates, K-12 youth and teachers, and the general public. Given the Center’s size, the logistics of engaging all members requires a broad menu of opportunities, simple systems for participation, a low barrier of entry, and organized supportive resources. The new team structure will further support this strategic goal.

* Programs uniquely led, organized, and/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 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). During 2015, support to recipient museums was completed for Pocket Tech –
replacing parts, etc. Additionally, the Penn State MRSEC-TFI partnership as a model for building museum kits to communicate current science was presented at the 2015 Association of Science-Technology Centers Conference. Lastly, work has been done to explore various options for the digital framework of the next museum kit project, a digital resource that synthesizes previously created content into a meaningful, self-directed learning opportunity about materials science for students, teachers, and families. Options include the creation of an independent app or tying into existing platforms. Another consideration is whether to design for a hand-held device or an interactive website. A final choice will be made at the first planning meeting in early 2016.

Public Outreach Events

The Penn State MRSEC continued much of its traditional involvement in multiple public outreach events during the reporting period of November 1, 2014 – October 31, 2015.

*NanoDays™ at Penn State*: (March-April) As a recipient of the 2015 NanoDays kit from NISE Net (Nanoscale Informal Science Education Network), the MRSEC organized and hosted three events. Local partners included Discovery Space of Central PA, Materials Research Institute (MRI), Center for Nanotechnology Education and Utilization (CNEU), and Center for Science and the Schools (CSATS).

- **NanoDays at Discovery Space (March 28, 2015)**: At the local Discovery Space of Central PA children’s science museum, MRSEC volunteers teamed up with Penn State elementary education majors and upper-elementary youth from the museum’s Kids Advisory Board to prepare and present NanoDays kit activities to the public. 102 visitors attended.
- **Science Café (April 14, 2015)**: At a weekly research Café held at MRI, ~90 graduate students and faculty heard the personal testimony of a MRSEC graduate student who engages regularly in outreach and has gained many benefits in the process. NISE Net activities were presented at stations before and after the discussion.
- **Nanotechnology Workshop for Teachers (April 28, 2015)**: 22 Pennsylvania K-12 educators (1 upper elementary, 6 middle school, 13 high school, and 2 post-secondary; 11 males, 11 females) learned about nanoscale science and technology via a one-day workshop. Activities included faculty presentations, a tour of Penn State’s materials characterization and fabrication facilities, exploration of NISE Net activities with graduate students, remote access and control of a scanning electron microscope (SEM), an inquiry-based classroom-ready lesson titled, and information about post-secondary education and career opportunities in nano-related fields.
**Science at the Central Pennsylvania Festival of the Arts – Children & Youth Day**: (July 8th) Each summer, the local town and gown community hosts one of the largest arts festivals in the country, the Central Pennsylvania Festival of the Arts. On “Kids Day”, which precedes the official event, science takes over Old Main Lawn with booths featuring numerous hands-on activities. This year, 14 booths were coordinated by the Center, 9 of which were directly staffed by MRSEC-affiliated graduate students, faculty, and staff (20 volunteers in total) who worked in teams with 47 REU students and a diverse group of 37 Upward Bound Math and Science (UBMS) high school students. These multi-level, behind-the-table teams worked together to prepare their activities and presentations. The team structure provides a mentoring aspect to the event, which is fostered through preparation meetings prior to the event. Although engaging the children and families in front of the table is a primary goal, the impact is most strongly experienced behind the table, by the volunteers. Improved science communication is a frequently mentioned benefit, and positive interactions between volunteers also support recruitment and retention of high school and undergrad students in STEM. Grad leaders receive training ahead of time so that they are prepared for their leadership and organizational role. In 2015, one longtime MRSEC volunteer asked to take an even larger leadership role, and essentially organized the entire event herself with staff support. Despite a rainy day, visitor counts indicated that ~1100 children and adults engaged in the activities.

**Tours of the MSC**: The Millennium Science Complex (MSC) is the newest and largest research building on Penn State’s campus, and the home of Penn State’s Materials Research Institute (MRI). MRI user facilities include the Nanofabrication Lab, the Materials Characterization Lab, and the Materials Computation Center. Campus visitors often want to have a tour of the building; yet MRI staff responsibilities do not often permit them to be available to give tours. An industry liaison handles the industry tours, but many tour requests come from student groups, REU participants, visiting high school students, teachers, and interested alumni. Tours provide fantastic opportunities for graduate student professional development in science communication, recruitment and retention, and improved public awareness. An initial team of 6 MRSEC graduate students were recruited and trained to start giving MSC tours. These students led guided tours for over 400 individuals in the past year.

**GWIS National Meeting**: (June 19th) A group of 4 MRSEC faculty and graduate student volunteered hosted an education and outreach themed talk to ~20 attendees of the conference. The presentation highlighted the Franklin Institute partnership and the MRSEC-led NanoDays and Arts Fest Kids Day events, and was followed by examples of the interactive demonstrations and activities associated with these programs.
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.

Science-U – Science Leadership Camp*: (July 19th – 24th) Science Leadership Camp: Elements of Innovation is a weeklong residential summer camp experience attended by a diverse group of 30 high school aged youth (47% female; 20% URM). MRSEC sponsored 10 full scholarships* (4 females; 5 URM) and assisted with the recruitment and selection of applicants from underserved and underrepresented groups. Center faculty and graduate students hosted three out of the six groups of high school campers for a half-day, hands-on, lab-based “research snapshot” of their lab. MRSEC members also hosted the annual “scientist mixer” mentoring event. Moments from this successful event are showcased in a video, viewable online (https://www.youtube.com/watch?v=K7a4eWvu Tk). Summative and long-term follow-up camper evaluations both indicate that the camp effectively supports and guides students’ STEM career goals; one past camper wrote that “Attending the Penn State Science Leadership camp really shaped my interest in STEM related fields. It helped me to realize how important science is in our society, and that I wanted to dedicate myself to one of the STEM-related fields.”

Summer Experience in the Eberly College of Science (SEECoS) & College of Earth & Mineral Sciences (SEEMS): (Summer 2015) The lab groups of three MRSEC faculty (Long-Qing Chen, Thomas Mallouk, and Joan Redwing) each mentored 2 or 3 high school students from the Upward Bound Math and Science (UBMS) program (serving low-income and first generation students from underrepresented and underserved populations in PA) for a six-week research-based project. A full day Symposium with faculty questions and feedback on student presentations concluded the event.

Higher Achievement: (August 5th) MRSEC continued its annual support of this program by presenting two sessions of “Are smart phones really smart?” to a total of ~40 girls and boys in the 7th-8th grades (the majority of whom are first-generation college-bound students).

Research Experiences for Undergraduates and Teachers

Research Experiences for Undergraduates (REU): The Center (DMR-1420620) worked alongside the Physics Department to recruit 28 participants for the Interdisciplinary Materials & Physics REU program (DMR 1062691). Of these, 9 were funded directly through the Center (including 1 Millennium Scholar from Penn State), 11 were funded via the REU site grant, and the remaining 8 were supported from other sources. The 9 MRSEC funded students were:
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<tr>
<th>REU Student</th>
<th>College/University</th>
<th>Faculty Mentor</th>
<th>Research Project Title</th>
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<tr>
<td>Forrest Brown</td>
<td>Georgia College</td>
<td>Venkatraman Gopalan</td>
<td>Symmetry and Structural Investigations of HRTiO4 (R=Sm, Eu) Compounds at Low Temperatures</td>
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<tr>
<td>Kursti DeLello</td>
<td>University of Central Florida</td>
<td>Joshua Robinson</td>
<td>Opto-Electrical Modulation of Van der Waals Solids via Metal-to-Insulating Transition Substrates</td>
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<td>Christopher Bernard Rodriguez</td>
<td>University of Puerto Rico at Cayey</td>
<td>Scott Phillips</td>
<td>Development of a depolymerizable polymer that responds when exposed to specific stimuli giving amplified responses</td>
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<td>Gabriel I. Vega Bellido</td>
<td>University of Puerto Rico Mayaguez</td>
<td>Tom Mallouk</td>
<td>Chemotactic Interactions of Glucose Oxidase and Catalase Based Micromotors</td>
</tr>
<tr>
<td>Olivia Vilella¶</td>
<td>Penn State University</td>
<td>Mauricio Terrones</td>
<td>Synthesis of Interconnecting Graphene Oxide and Carbon Nanotubes through Hydrothermal Reaction and Chemical Vapor Deposition</td>
</tr>
<tr>
<td>Karina Keefe</td>
<td>University of Maryland Baltimore County</td>
<td>Joshua Robinson</td>
<td>CVD and Epitaxial Graphene Growth and Characterization</td>
</tr>
<tr>
<td>Ryan Katona</td>
<td>Lynchburg College</td>
<td>Vin Crespi</td>
<td>Reconfigurable arrays of bistable graphene nanocones created through topological defects</td>
</tr>
<tr>
<td>Wei Trinh</td>
<td>University of Maryland Baltimore County</td>
<td>Long-Qin Chen</td>
<td>Combined Experimental and Numerical Method for Designing High Temperature Metalized Thin Film Polymer Capacitors</td>
</tr>
<tr>
<td>Jeffrey Mohan</td>
<td>McGill University</td>
<td>Noel C Giebink</td>
<td>Luminescent cooling of organic molecules in the solid phase with optical enhancement</td>
</tr>
</tbody>
</table>

¶ Millennium Scholar

MRSEC faculty also served as mentors for 12 of the 19 remaining participants:

<table>
<thead>
<tr>
<th>Faculty Member</th>
<th>Student</th>
<th>College/University</th>
<th>Research Project Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitin Samarth</td>
<td>Alexis Bowers</td>
<td>Lock Haven University of Pennsylvania</td>
<td>Magneto-Optical Study of Lithographically Patterned Ferromagnetic Multilayer (Co/Pt)8 Micro-Channels</td>
</tr>
<tr>
<td>Susan McKinstry</td>
<td>Leonard Jacques</td>
<td>University of Maryland, Baltimore County</td>
<td>Growth of IrO2 Thin Films</td>
</tr>
<tr>
<td>Mauricio Terrones</td>
<td>Steven Lippold</td>
<td>Clarion University of Pennsylvania</td>
<td>Growth and Micropositioning of 2-D Layered Materials</td>
</tr>
<tr>
<td>Qi Li</td>
<td>Joshua Schulz</td>
<td>Geneva College</td>
<td>Effect of Growth Temperature on the Diameter, Length, and Morphology of Bi2Te3 Nanotubes</td>
</tr>
<tr>
<td>Darrell Velegol</td>
<td>Lazaro Pacheco</td>
<td>Rutgers University</td>
<td>Enhancing the Fouling-Resistance of Reverse Osmosis Membranes</td>
</tr>
<tr>
<td>Name</td>
<td>Institution</td>
<td>Research Topic</td>
<td></td>
</tr>
<tr>
<td>-----------------------</td>
<td>------------------------------------</td>
<td>---------------------------------------------------------------------------------</td>
<td></td>
</tr>
</tbody>
</table>
| Chris Geibink         | Loyola University Chicago          | Optimizing Charge Transfer State  
|                       |                                    | Electroabsorption in Planar Heterojunction  
|                       |                                    | Organic Photovoltaics                                                             |
| Peter Butler          | Polytechnic University of Puerto Rico | Red Blood Cell Membrane Fluctuations                                               |
| Venkat Gopalan        | Pacific Lutheran University, Washington | Crystalline germanium optical fibers for low-loss mid-infrared semiconductor waveguides |
| Ayusman Sen           | Virginia Commonwealth University   | Synthesis and Movement of Catalytically powered Janus motors                       |
| Mauricio Terrones     | Iberian-American University        | Carbon nanotube enhanced Graphene Oxide  
|                       |                                    | Macroscopic-hybrid Films by Dry Film Scrolling Method                             |
| Eric Hudson           | Penn State University              | The Effects of Acoustic Noise On Scanning Tunneling Microscopy                     |
| Nitin Samarth         | Penn State University              | Photocurrent Generated by Circularly Polarized Light in Magnetically Doped Topological Insulators |

Students participating in the REU program engaged in cutting-edge materials science research, with access to state-of-the-art facilities and exposure to interdisciplinary collaboration at Penn State. Participants took part in a number of professional development opportunities, including diversity awareness, science communication training, a visit to the Franklin Institute, public outreach at “Arts Fest Kids Day”, and presentation at the Summer Research Symposium, an event modeled after a large professional conference. Students also attended weekly seminars to broaden their interdisciplinary skills and learn about career opportunities within the field.

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 (Christine Keating, Joshua Robinson, Joan Redwing, Qi Li, and Susan Trolier-McKinstry) were advisors for participants in the NNIN REU program.
- Two faculty members (Tom Mallouk and Suzanne Mohney) were advisors for participants in the PPG funded summer research program.
- Two faculty members (Joan Redwing and Suzanne Mohney) were advisors for participants in the 2D & Layered Materials summer research program.
- Two faculty members (Tony Huang and Ali Borhan) supervised students in the biomaterials focused Chemical Engineering REU program.

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.

**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), the MRSEC provided multiple avenues of support for the RET program. Participants received 3.5 graduate credits from Penn State, as well as 30 hours of Pennsylvania Act 48 credit. Support from the MRSEC included faculty advisor participation, funding for project materials, and staff support for preparing presentations at the Summer Research Symposium.

The objective of the six-week RET program at Penn State is to give participating STEM teachers the opportunity to engage in hands-on research in materials science and nanotechnology under the mentorship of a faculty mentor. Teachers who have engaged in hands-on science are better equipped to develop curriculum and materials that support STEM education. Participants in the RET program worked collaboratively to develop lesson plans, research presentations (oral and poster), and papers for publication. In addition, participants established collaborative relationships with MRSEC faculty members. These relationships guide K-12 teachers in impacting STEM education by providing both in-service and pre-service teachers with content, experience and knowledge on careers in materials science. Following completion of the summer RET program, participating teachers are also encouraged to apply for a mini-grant to augment their K-12 STEM efforts using knowledge gained in the RET program.

Nine teachers participated in the 2015 RET program via NSF funding through the MRSEC (3), the REU site grant (3), and two supplementary NSF grants from Center faculty (3). Of these, only one site-grant-funded teacher was in a non-MRSEC lab. The following 8 teachers were all hosted by current 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>Steven Schulz</td>
<td>Manheim Township High School</td>
<td>Ayusman Sen</td>
<td>Chemical Manipulation of Silver Phosphate Micromotors</td>
</tr>
<tr>
<td>Stephen Stilianos</td>
<td>Somerville High School</td>
<td>Paul Cremer</td>
<td>Exploring the Hofmeister series with PNIPAM</td>
</tr>
<tr>
<td>Douglas Schunk</td>
<td>State College High School</td>
<td>John Badding</td>
<td>Under Pressure - Phase Change Demonstrations</td>
</tr>
<tr>
<td>Sandy Ranstead</td>
<td>Bina High School</td>
<td>Christine Keating</td>
<td>UV-absorbance of C-Phycocyanin potentially as a-sunscreen pigment</td>
</tr>
<tr>
<td>Name</td>
<td>School/Department</td>
<td>Co-likes</td>
<td>Project</td>
</tr>
<tr>
<td>----------------------</td>
<td>-----------------------------------</td>
<td>---------------------------------</td>
<td>-------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Robert White</td>
<td>State College High School</td>
<td>Qi Li</td>
<td>The Effect of Sodium Hydroxide Concentration on Tellurium Nanowire Length and Morphology</td>
</tr>
<tr>
<td>Mark Yeckley</td>
<td>Glendale School District</td>
<td>Christine Keating</td>
<td>ZnO Friend or Foe? Nano Particles, Big Deal!</td>
</tr>
<tr>
<td>Martha Dombroski</td>
<td>St. Rose of Lima School</td>
<td>Christine Keating</td>
<td>Does Sunscreen = Protection from the Sun’s Harmful Rays? You Do the Math!</td>
</tr>
</tbody>
</table>

**Evaluation & Assessment**

Evaluation and assessment efforts of education and outreach initiatives are part of every MRSEC program listed above. Metrics and tools are designed separately for each program, depending upon particular goals and desired outcomes, and implemented accordingly. Assessment methods include participant and volunteer surveys, team-based inquiry, behavioral observations of attendees, instruments utilized within activities, formal and informal interviews, etc. Collecting and maintaining accurate records of audience demographics and volunteer contributions remains a Center priority. All collected information is reviewed during post-program wrap-up efforts and summarized to evaluate the impact on volunteers and participants, as well as identify program successes and needed changes. Given the new “MRSEC Outreach Team” structure, the evaluation and assessment of the graduate student volunteer experience and professional development is of particular interest for the coming year.
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-
Postdoctoral Mentoring Plan

In addition, research-focused 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, including the unique considerations behind successfully managing synthesis/experiment/theory projects. 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 postdocs from the past award period 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. The most recent postdoctoral researchers have encountered comparable success to this cohort.

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 secured permanent teaching positions, and our prior instructor-level education/outreach manager is now an associate dean. We have developed a mentoring plan for the current Education/Outreach postdoctoral fellow (Sydney Chamberlain) that includes continued research activities, opportunity to co-teach an interactive hands-on undergraduate physics course, and deep engagement in MRSEC educational activities in close collaboration with experienced MRSEC staff and faculty. 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 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. Outcomes from these meetings include renewed focus on enhancement of spoken and written English skills by giving the postdoctoral researcher responsibility to lead regular project meetings, opportunity to develop new experimental skills through collaboration on electron microcopy and independent development of laser systems, guided experience in proposal writing, additional opportunities to present at conferences, and combined collaborative opportunities in both first-principles theory and experiment with multiple groups.
8. Center Diversity – Progress and Plans

*Diversity Strategy Overview:* The Center’s approach to diversity is guided by the following four principles: (1) seek to recruit and engage underrepresented individuals as participants in all Center activities and programs; (2) maintain a balanced portfolio of diversity-focused initiatives that target audiences at multiple academic levels (high school through graduate school) and incorporate vertical mentorship whenever possible; (3) connect outreach and educational efforts with direct involvement in Center research, or a pathway towards potential future Center membership; and (4) build and utilize collaborative partnerships to produce greater results and reach stronger target audiences than can be accomplished or reached otherwise. Applying these principles to the graduate admissions processes of member departments is a particular focus, along with recruitment and retention efforts that support it. It is well known that complex factors attract and retain underrepresented students and faculty, and these can be challenging to identify and surmount. As a result, Center staff and faculty are intentionally building strong working relationships with the Director of the Millennium Scholars program (Starlette Sharp M.S.), the Senior Director of the Office of Graduate Educational Equity Programs (OGEEP, Dr. Stephanie Preston), member department Diversity Chairs, and the college-level multicultural officers. A Diversity Committee (comprised of Center leadership and faculty, outreach staff, partner program representatives, member department representatives, and multicultural officers) oversees and assists with the implementation of diversity initiatives.

*Current Status and Progress of Center Participation:* The following tables summarize the current status of diversity engagement efforts in research activities.

<table>
<thead>
<tr>
<th>MRSEC Participants 2015</th>
<th>Total</th>
<th>Women</th>
<th>Underrepresented Minorities (URM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Faculty</td>
<td>45</td>
<td>10 (22%)</td>
<td>3 (7%)</td>
</tr>
<tr>
<td>Postdocs</td>
<td>11</td>
<td>1 (9%)</td>
<td>0</td>
</tr>
<tr>
<td>Graduate Students</td>
<td>59</td>
<td>20 (34%)</td>
<td>4 (7%)</td>
</tr>
<tr>
<td>REU (Undergraduates)</td>
<td>20</td>
<td>8 (40%)</td>
<td>8 (40%)</td>
</tr>
<tr>
<td>RET</td>
<td>10</td>
<td>2 (20%)</td>
<td>0</td>
</tr>
</tbody>
</table>

*Table 1: Summary of 2015 participants by category of Women and Underrepresented Minorities (URM)*

*Research Experiences for Undergraduates (REU):* A diverse group of students was recruited for Penn State’s *Interdisciplinary Materials & Physics REU*. Of the 28 total participants, 20 were funded by NSF via the MRSEC (9 students) + REU (11 students) site grant (DMR 1062691). These NSF funded students included 8 (3+5) women and 8 (3+5) URM individuals. In preparation for summer 2016, recruitment efforts during fall 2015 included visits to UMBC Meyerhoff and the Society for Advancement of Chicanos/Hispanics and Native Americans in Science
(SACNAS) conference. (The SACNAS booth was a MRSEC-wide coordinated effort by the MRSEC Education Network.) Further, eligible attendees at the Penn State STEM Open House received information about all Penn State summer research programs. MRSEC faculty have also continued to strengthen ties with Penn State’s new *Millennium Scholars* program, modeled after the very successful Meyerhoff Scholars program at University of Maryland, Baltimore County (UMBC). These diverse science and engineering scholars are committed to the completion of a PhD. Thus far, 8 out of 35 Millennium Scholars (from Cohorts 1 & 2) have found homes in MRSEC faculty labs for their senior thesis. This is notable given the fact that each Cohort welcomes students across all science and engineering disciplines. Of these, 7 chose to spend their first or second summer at Penn State getting a strong start on their thesis project.

The Center-led summer program series titled *Different Science, Different People, Working Together* continued in 2015 with 113 total students on the roster for each joint event. Nine summer research programs participated, each with a distinct research focus. This joint series included a welcome orientation with diversity training and community-building activities, and a clear message about the importance of personal and professional diversity in STEM fields, as well as growing trends towards interdisciplinary research. Two additional seminars featured: *Science Communication: Communicating the Good News on Energy, the Environment, & Your Future* with Dr. Richard Alley (Penn State), and *Beyond the PhD: Career Pathways Ahead* with Dr. Thomas Fu (Office of Naval Research), Dr. Michael Makowski (PPG Industries, Inc.), and Dr. Amit Das (State of the Art, Inc.).

*Partnerships for Research & Education in Materials (PREM):* During 2015, the Center was the named partner in two successful PREM proposals for the first time, a culmination of sustained efforts by the Center in this regard. The first, North Carolina Central University (NCCU) includes a integrated research and education plan based upon three collaborative research thrusts and a seed project. Each summer, up to 2 master students and 4 undergraduates from NCCU will spend 10 weeks at Penn State. The undergraduates will participate in the *Interdisciplinary Materials & Physics REU*. Further, each NCCU undergraduate researcher (a rising junior or senior) will be matched with an upper-class Millennium Scholar as part of the “Penn Pal” peer-mentoring program. These pairs will meet regularly and attend various planned activities. At the end of the summer, which includes a symposium with short talks and a poster session for all REU students, the pair will jointly decide upon a second professional conference to attend together and present their posters. Younger NCCU PREM students will remain in North Carolina for the summer to begin building their research skills. Concurrently, they will be strongly encouraged to enroll and register for MatSE 201 “*Introduction to Materials*” - an online course offered by Penn State’s World Campus. Additional visits to both universities will occur throughout the academic year. To initiate the partnership, in-person planning visits to each university by the other have already occurred.
The second PREM, with Cal State L.A., focuses upon the establishment of a Master of Science Degree in Materials at CSULA, with research collaborations around three themes. Participation in summer research programs at Penn State by CSULA undergraduates (4) and master students (2) will also take place. An in-person visit by Penn State faculty and staff to CSULA is being planned for early 2016.

**Graduate Recruitment:** The third annual STEM Open House (initiated at a 2013 MRSEC Diversity Committee meeting and held annually with MRSEC support and participation on the planning committee) was held October 15-18th, 2015, led by OGEEP. A large increase in applicant numbers and academic quality caused the program to double in size. Attendees included 63 underrepresented and underserved minority undergraduate and female students in their junior or senior year, as well as post-graduate master’s students. The event provides a preview of Penn State STEM graduate programs well before the application deadline, 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 faculty hosted students for departmental visits, attended meals, gave presentations, and served as panelists. Institutional support has increased broadly and remained strong. OGEEP is currently in the process of compiling application, offer, acceptance, and retention data for the first three events.

**Diversity in K-12 Programs:** MRSEC supported scholarships for 10 high school campers from underserved areas (4 female, 5 URM) to attend a unique weeklong residential experience at Penn State’s Science Leadership Camp. Applicants were recruited through an expanding number of pipelines, as new connections are established with schools and Trio programs that serve minority and economically disadvantaged communities. Further, three MRSEC faculty hosted Upward Bound Math & Science (UBMS) students in the Summer Experience in the Eberly College of Science (SEECoS) program to do research project in their labs. All UBMS students were also placed in multi-level teams with Physics/MRSEC REU and MRSEC graduate students for a full day of science outreach at the annual local Arts Festival Kids Day event. (See Section 6; For UBMS info: http://equity.psu.edu/ubms/pdf/2015-summer-stem-academy-exec-summary)

**Plans for the next reporting period:** The Center will further develop and grow several seedling diversity initiatives. (1) A MRSEC-Sloan Scholars partnership via OGEEP will bring up to 5 new minority and/or female graduate scholars into Center research activities. (2) The MRFN Faculty Speaker Series will foster mutual exchanges between Center and MSI faculty to pursue potential research collaborations. (e.g. Starlette Sharp has initiated the interest of two faculty at Tuskegee University.) (3) The two new PREM partnerships with NCCU and Cal State LA will be ramped up. These initiatives are intended to increase the diversity of Center research participants, support institutional level graduate student recruitment efforts, and create, as well as strengthen, relationships with new and existing MSI partners.
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. One of the important vehicles for collaboration with industry is the MRSEC’s Industrial Affiliates Program, now in its seventh 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.

Collaborations of MRSEC Faculty with Industry and National Labs:

Susan Trolier-McKinstry is collaborating with Murata on epitaxial integration of perovskite oxides on silicon, and also have relationships with Xaar, the Center for Dielectrics and Piezoelectrics (23 companies), Dow, eXo, UTRC, Intel, and Texas Instruments.

Roman Engel-Herbert is collaborating with Argonne National Lab to install a hybrid MBE growth reactor on a beamline for in-situ real-time growth experiments.

Long-Qing Chen is collaborating with researchers at Oak Ridge National Lab (Sergei V Kalinin), Los Alamos National Lab (Quanxi Jia) and Sandia National Lab. Venkat Gopalan is collaborating with researchers at Oak Ridge National Lab and Argonne National Lab (H. Wen, J. Freeland, M. Holt).

James Rondinelli will deliver a tutorial talk at the 2016 Spring MRS Meeting on Designing Layered Complex Oxides, which is aimed at graduate level students and professional scientists aiming to gain a deeper understanding of the field.


IRG researchers in acoustically powered systems are currently engaged in collaboration with several companies on developing products related to acoustic motors and acoustic tweezers, including Ascent Bio-Nano Technologies, Johnson & Johnson, Pfizer, Milli-
pore, Druker Diagnostics, Zimmer-BioMET, Malvent Instruments, and Genefluidics.
Prior work in the IRG related to the action of chemically powered pumping in georeservoirs has now evolved into a project in collaboration with Halliburton on pseudomorphic mineral replacement reactions in georeservoir materials, by ‘chemical-mechanical fracking’.

IRG3 members have started a collaboration with IBM to measure the band structure of advanced materials relevant to next-generation electronics and photovoltaics, with a long-term student visit at IBM and reciprocal visits at MRSEC-supported labs.

In-operando x-ray diffraction studies were conducted on the 2-ID-D beamline at the Advanced Photon Source at Argonne National Laboratory in work with IRG4. Multi-dimensional characterization of the electrically triggered phase transition in vanadium dioxide was performed using X-ray diffraction spectroscopy at nanoscale resolution. The evolution of the crystal structure was spatially and temporally mapped across two terminal devices during electrically induced phase transition.
10. International Activities

The Penn State MRSEC has a substantial international component to its research and outreach program. The research program in IRG3 benefits from a deep and long-term relationship with the University of Southampton. Seed efforts in topological systems have strong connections to China, particularly since several MRSEC alumni have taken up permanent positions there. IRG2’s work on ultrasonically powered motors is proceeding in part through interactions with collaborators in France and Dundee, with additional theory connections to the UK. IRG1 also has several important relationships with international collaborators. Specific international activities in the past year include the following:

- V. Gopalan in IRG1 is collaborating with Anna Morozovska, and Eugene Eliseev in the Ukraine on ferroelectric theory.
- L. Q. Chen in IRG1 is collaborating with C. W. Nan, in Tsinghua, China on multiferroic theory.
- IRG2 hosted international visits from research collaborators Mauricio Hoyos, Wei Wang, Sandy Cochran, and Ramin Golestanian.
- Prof. Mario Pantoja from the University of Granada, Granada, Spain, is currently a visiting professor at Penn State working with Prof. Douglas Werner in IRG4 on developing efficient computational modeling techniques for nanoloop antennas/resonators. Both analytical and numerical models are under development for individual nanoloops as well as coupled arrays of nanoloops. Prof. Werner plans future visits to the University of Granada as part of the collaboration.
- Dr. Xiaobin Fan from Tianjin University spent a sabbatical year in the Mallouk lab working on the chemistry of transition metal dichalcogenides, in association with MRSEC Seed efforts.
- An international collaboration with John Hayes and Pier J.A. Sazio of the Optoelectronics Research Center of the University of Southampton in UK and a MRSEC Seed project used a silica capillary from Hayes and Sazio as a template for a 150nm diameter and 6mm long gallium-indium eutectic nanowire, demonstrating the possibility to trapping individual fluxons and observe resistance switching in the wire (Nano Lett. 15, 153–158 (2015)).
- The MRSEC continues to collaborate with Professor Mingliang Tian of the High Magnetic Field Laboratory of China, recently completing a study of surface superconductivity in a bismuth nanowire (Nano Lett 15, 1487–1492 (2015)).
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. The MRSEC 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. 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 Computation Center (MCC), a University-wide facility providing education, support and research activities to help users incorporate simulation into their research programs, through contributions towards computational hardware. The MCC sponsors short courses and workshops on simulation/modeling software on a regular basis. The MCC also hosts user group meetings organized around particular types of simulation, including, the Density Functional Theory User Group.

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, and are managed 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.

MRSEC equipment acquisitions in 2015 have focussed on key resources needed to meet the needs of the constituent IRGs and also positively impact the larger materials research community. The Gopalan group revamped their ultrafast laser lab by purchasing a new laser system from spectra physics with 6W output power, and wavelength tuning out to 15 microns. The MRSEC contribution was leveraged by DMR-1210588, and DMR-1107894 as well. This upgrade is critical to IRG1 and is also of great use to IRGs 3 and 4 (Badding, Giebink, etc.). Its placement in a shared facility makes it available more broadly to support work on infrared materials, topological photonic crystals, ultrafast thermal conductivity measurements, THz spectroscopy, nonlinear polymer composites, etc. In addition, the MRSEC supported the acquisition of key pieces of supporting infrastructure for the double aberration corrected Titan microscope, including a PIPS II ion mill that is critical for the preparation of extremely thin TEM samples with minimal damage for atomic-resolution imaging and elemental mapping of many materials and a dual EELS upgrade for the Titan S/TEM to enable the measurement of subtle chemical shifts and bandgaps with better than 0.2eV energy resolution. It also allows researchers to map specimens according to chemical state with sub-nm resolution. Finally, a MRSEC contribution towards a heavily used shared-use Raman microscope provides state-of-the-art micro-Raman capabilities spanning UV-Vis-NIR, with ultra-low frequency filters and coupled to a TERS capable scanning probe microscope coupled to the microscope.

The MRSEC partners with the Materials Research Institute to deliver the MRFN Faculty Fellowship Program summer program. This program is targeted towards establishing relationships between the MRFN and faculty from Primarily Undergraduate Institutions. The program bolsters faculty research programs by providing the resources necessary to utilize advanced materials characterization facilities at Penn State. In 2015 the program grew out of "summer" mode to become a year-long fellowship. This modification has enable fellows to work beyond the summer months and involve more student in visits to Penn State. The average award amount in 2015 was ~$3000, this reduction from years past enabled us to expand the program to meet growing interest. In 2015 we receive a record 19 proposals from more than 10 different academic institutions. The quote below from Kate Plass, a fellow initially funded in 2014, exemplifies the positive impact of the program.

“The MRFN program was a gateway to the inviting PSU community. Giving a MRSEC seminar was a great introduction to interested faculty and resulted in some joint experiments. It has also lead me to spend my sabbatical learning heterodimer synthesis, ion exchange reactions, and characterization techniques in the Schaak lab. This has opened up new pathways for research with my students and in collaboration with the Schaak lab. Embedding in the PSU chemistry department has allowed further opportunities to network with visiting seminar speakers."
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 Gopalan, the IRG leaders (Gopalan, Sen, Badding and Keating), the Penn State Materials Research Institute (MRI) Director Clive Randall, Outreach Director Dreyer, Mohney, Central Facility Lab director Chan, and ARL representative Donnellan. Mallouk oversees the outreach portfolio. The Executive Committee is well connected to University administration in materials research through Randall and Trolier-McKinstry (who is also co-Director of the Penn State Nanofabrication Facility and also a member of the executive committee), 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 bi-monthly, typically after the weekly MRSEC Seminar (or sometimes electronically). 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. During the ramp-up of the two new IRGs, the MRSEC Director is engaging with IRG leaders Badding and Keating on a regular basis to monitor the initiation of these efforts and to anticipate any emergent needs.

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
Administration and Management

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 Eric Hudson (Chair), Mallouk (Associate Director), Ron Redwing, Sydney Chamberlain (Educational Outreach Coordinator), Kristin Dreyer (Educational Outreach Manager), Hank McCoullum (Diversity 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 is now placing particular focus on the launching of the two new PREM partnerships and the growth of the Millennium Scholar program.

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). Since the NSF second year review is happening fairly early in the second year, the next visit of the EAC will be scheduled to occur early in year 3.

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-advice them. 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 next project review is scheduled for early 2016, which will provide an opportunities to adjust strategic
priorities as the new research efforts proposed in the renewal competition complete their first full year of support.

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 Executive Committee and Institute directors provide written reviews and if necessary meet 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 additional 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 independently funded as a group collaboration.

**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. Kristin Dreyer is Outreach Director. Postdoctoral fellow Sydney Chamberlain 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 Randall, together with David Fecko, who oversees industrial outreach within the Materials Research Institute and reports directly to Randall. 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 2014 / 2015

Ahmad Ahsan Nawaz, Ph.D., Fall 2014, National University of Sciences and Technology (NUST), Pakistan

Suzanne Ahmed, Ph.D. Summer 2015, Merck

Wentao Duan, Ph.D., Spring 2015, Pacific Northwest National Lab (PNNL)

Craig Eaton, Ph.D currently working at Intel Corporation

Yijia Gu (Ph.D. Penn State, December 2014; ALCOA)

Abhishek Kar, Ph.D., Spring 2015, Shell Oil

David Kirby, Ph.D in Chemistry, he is currently a Lecturer in Chemistry at Penn State Behrend

Ding Ma, Ph.D in Electrical Engineering, working in Shanghai, China

Francelys Medina, postdoc, teaching at Penn State Dubois Spring 2016

Nicolas Polivert, postdoc working at Baylabs in California

Gregory Stone postdoc, Penn State, working at the Picattnny Arsenal Army research labs

Megan Strayer, Ph.D., Penn State, teaching in Chemistry at Duquesne University

Junjie Wang, Ph.D in Physics, working at Global Foundries

Fei Xue, Ph.D, Penn State, Continuing as a Postdoc in Prof. Chen’s group

Vinita Yadav, Ph.D., Spring 2015, Dow Chemical

Di Yi: finished PhD, Berkeley; currently postdoc at Stanford

Yanhui Zhao, Ph.D., Fall 2014, Intel
14. Publications and Patents

**IRG 1**

**a. Primary Support**


**b. Partial Support**


IRG 2

a. Primary Support


b. Partial Support


IRG 3

a. Primary Support

b. Partial Support

IRG 4

a. Primary Support

Boehm, S. J.; Lin, L.; Guzmán Betancourt, K.; Robyn Emery, R.; Mayer, J. S.; **Mayer, T. S.**


b. Partial Support


**Seed – Superconductivity and Fluxon Trapping in Long Nanowires**

a. Primary Support


b. Partial Support


**Patents**

**IRG 2**

**Tony Huang Patent Applications**

“Separation of low-abundance cells from fluid using surface acoustic waves” (U.S. Patent Filing, 62/035926)

“Acoustic manipulation process and acoustic manipulation device” (U.S. Patent Filing, 62/205,871)

“System and method having an SAW substrate and a removable container” (U.S. Patent Filing, 62/245,491)

**Ayusman Sen Patent Application**

15. New Investigators

None to report.
16. Honors and Awards

Arjun Agrawal Thesis Prize by Lambda Chapter of Phi Beta Kappa, Douglas G. and Regina C. Evans Award for Research Achievement 2015.

John Badding received the Faculty Scholar medal in Physical Sciences, awarded at Penn State annually to one faculty member in the physical sciences.


Long-Qing Chen, American Ceramic Society Fellow, October 2015.

Yuchao Chen, Penn State Alumni Association Dissertation Award 2015.

Yuchao Chen, Thomas and June Beaver Award, The Pennsylvania State University 2015.

Yijia Gu, Chen group, April 2015, Chinese Government Award for Outstanding Self-Financed Students Abroad.

Ismaila Dabo, Ralph E. Powe Junior Faculty Award, Oak Ridge National Laboratory 2014.

Craig J. Fennie, fellow of the APS 2015.


Tony Huang: The Huck Distinguished Chair in Bioengineering Science and Mechanics, Penn State University; Fellow, American Institute for Medical and Biological Engineering (AIMBE); Fellow, American Society of Mechanical Engineers (ASME); Fellow, Royal Society of Chemistry (RSC); Fellow, Institute of Physics (IoP)

Gerald Mahan, 2015 Lifetime Achievement Award for the International Thermoelectrics Society, July 2015.

Thomas Mallouk was elected to the National Academy of Science in April 2015.

Margaret Murnane, Honorary Degree of Doctor of Science, Uppsala University, Sweden 2016; Honorary Degree of Doctor of Science, National University of Ireland 2015; Elected to Member, American Philosophical Society 2015; Honorary Degree of Doctor of Science, University of College Dublin and Honorary Degree of Doctor of Science, Trinity College Dublin 2015.

Nitesh Nama, Third-Place Prize in Paper Competition at the ESM Today Graduate Research Symposium 2015.

Nitesh Nama, Sebro Scholarship, The Pennsylvania State University 2015.
Ramamoorthy Ramesh, Berkeley, 2014 TMS Bardeen Prize
Ramamoorthy Ramesh, Berkeley, 2014 Thomson Reuters Citation Laureate
Ayusman Sen: Elected Fellow, Royal Society of Chemistry 2015
Susan Trolier-McKinstry, MRS Fellow 2015.
Susan Trolier-McKinstry, elected to MRS Vice President 2015.
Darell Velegol: Inaugural “World Class Engineering Professor” in the Penn State College of Engineering in April 2015.
Vinita Yadav, Baxter Young Investigator 2014.
Transition metal oxides offer properties beyond conventional semiconductors, but to bridge the gap between fundamental research and commercial devices requires wafer-scale growth of high-quality thin films. A novel combinatorial growth process developed by Penn State has produced the first wafer-sized thin films of near-stoichiometric vanadium dioxide VO$_2$. When the V:O ratio is exactly right, the material shows a four order-of-magnitude change in resistance across the wafer, enough to enhance state-of-the-art transistors and benefit non-volatile memory technology.

“Electronic grade” transition metal oxide films on a large scale can now be extended to other multivalent oxide systems.

Oxynitrides are attractive due to a combination of visible-light absorption, photocatalytic activity, and high dielectric permittivity. Their synthesis typically requires high-temperature NH$_3$ treatment of oxides, but the highly reducing conditions and the low mobility of N$_3^-$ greatly constraint the composition, structure, and hence properties of the resulting oxynitrides.

A MRSEC team has demonstrated a \textit{topochemical route} to making oxynitrides at less than 500°C using a perovskite oxyhydride as a host, obtaining a room-temperature ferroelectric BaTiO$_{3-x}$N$_{2x/3}$. Anion exchange is accompanied by a metal-to-insulator cross-over via mixed O–H–N intermediates. This “labile hydride” strategy can now be applied to other oxynitrides and perhaps other mixed anionic compounds. BaTiO$_{3-x}$N$_{2x/3}$ also has potential applications in next-generation electronics.
MRSEC-supported researchers have developed a reusable microfluidic device based on “acoustic tweezers” that can sort and manipulate cells and other micro/nanometer scale objects, potentially making biomedical diagnosis of diseases cheaper and more convenient in regions where medical facilities are sparse or cost is prohibitive. The team has found a way to separate the fluid-containing part of the device from the much more expensive ultrasound-producing piezoelectric substrate, which makes disposable acoustic tweezers possible.

Yuliang Xie, Sixing Li, James Lata, Liqiang Ren, Zhangming Mao, Baiyang Ren, Mengxi Wu, Adem Ozcelik and Tony Huang, Lab on a Chip, 2015. NSF DMR-1420620 (with additional support from NIH).
MRSEC researchers have used geometric boundaries to steer self-propelled Janus micromotors. The rotational diffusion of Janus micromotors around an axis perpendicular to the boundary is quenched by hydrodynamic interactions, which constrain a particle to move long distances along the boundary. The team has also for the first time measured the surface charge on these motors and quantified the electrostatic effects that govern their motion. Autonomous directed propulsion in the face of Brownian randomization makes possible applications of autonomous motors for cargo transport, drug delivery, sensing, environmental remediation, and micro-surgery that targets individual cells.
Amorphous silicon wires embedded in silica templates by high-pressure chemical vapor deposition (a technique also used to create ordered 3D metalattices) can be crystallized by a laser. Modeling reveals that shrinkage of the amorphous silicon upon crystallization creates extreme strain in these wires. A combination of experiment and theory suggests that the band gap can change by nearly a factor of two due to this strain. It may thus be possible to employ the technologically versatile silicon platform for detectors that function at near IR to mid IR wavelengths.
A current passed through VO$_2$ destabilizes the monoclinic semiconducting phase and induces a phase transition to the tetragonal metallic phase. While the electronic transition to the low resistance state is very fast, a complex and unexpected spatially varying structural distortion pattern is detected, lagging behind the electronic transition. These “structural aftershocks” reveal a complex interplay of electronic and structural phase transitions in VO$_2$ on ultrashort time scales in a device configuration which is of high relevance for newly proposed low power logic devices, such as hyper-FETs (10.1038/ncomms8812) or VO$_2$ oscillator based non-Boolean computing (10.1038/srep04964).
A single superconducting flux quantum or “fluxon” $\Phi_0$ with magnetic moment “↑” can be exploited to switch the resistance of a nanowire between two discrete values, with potential long-term application in creating new switching devices. The MRSEC team has produced extraordinarily long nanowires of superconducting Ga-In eutectic – centimeters in length – who extreme length assists in the formation of spontaneous Ga nanodroplets along the length of the nanowire with the right geometry to capture magnetic flux. Fluxons can be inserted or flipped by careful manipulation of magnetic field or temperature, to produce many metastable states each with different electron transport properties.

DMR-1420620 W. Zhao$^1$, J. L. Bischof$^1$, J. Hutasoit$^1$, X. Liu$^1$, T. C. Fitzgibbons$^1$, J. Hayes$^2$, P.A.J. Sazio$^2$, C. Liu$^1$, J. K. Jain$^1$, J. V. Badding$^1$, and M. H. W. Chan$^1$. Nano Letters 2015, $^1$Penn State, $^2$Southampton.
Integrating Diversity Across Programs

**Center diversity efforts:**

- Recruit and engage underrepresented individuals as participants in all Center activities and programs
- Target audiences at multiple academic levels and incorporate vertical mentoring
- Connect outreach efforts to involvement in Center research, or a pathway towards future Center membership
- Partner to produce stronger results and reach larger target audiences than can be accomplished otherwise.

**Arts Festival Kids Day**
Grads work in multi-level teams with REU and Upward Bound Math & Science volunteers to communicate science to kids and parents.

**Partnerships & Pipelines**
Efforts to build connections between research and education have yielded results with Penn State Millennium and Sloan Scholar programs, two successful PREM partners (NCCU & CSULA) and new diversity recruitment opportunities.

**Undergraduate Research**
MRSEC-led programs include diversity training, science communication and career path talks, and activities to create a cohesive, welcoming university-wide summer research community.

**Science Leadership Camp**
MRSEC hosts “research snapshots” and a scientist mixer, and sponsors at least 10 scholarships for campers who represent minority groups in STEM.

**STEM Open House**
The 3rd annual diversity grad admission event demonstrated MRSEC’s impact to support institutional change. The 2015 event doubled in size with attendees having strong undergraduate research experiences and GPAs.

**STEM Open House**
Penn State STEM Open House October 15-18, 2015

**STEM Open House**
The Millennium Science Complex (MSC) is the newest and largest research building on the Penn State University Park campus, and the home of Penn State’s Materials Research Institute (MRI). MRI user facilities include the Nanofabrication Lab, the Materials Characterization Lab, and the Materials Computation Center. Frequent requests for tours are received, but job responsibilities rarely allow the time needed for MRI staff to give them. An industry liaison person handles tours for potential industry partners and individual faculty provide personal tours for collaborators, but tour requests from student groups, REU participants, visiting high school students, teachers, on-campus conference attendees, and interested alumni are difficult to arrange due to a shortage of guides. Fortunately, these groups are perfect audiences for young researchers to meet and engage!

As a result, a MRSEC Tour Guide Team was piloted in 2015 with an initial team of 6 MRSEC graduate students to fill the need. Scripts were created, guides were trained, signage and props were utilized, and feedback from both guides and visitors was obtained. The result was successful. Tours take approximately 60 minutes and provide fantastic opportunities for professional development in science communication, recruitment and retention encouragement, and improved public awareness. Over the course of the year, these graduate students lead tours for over 400 individuals. In the process, special tour opportunities arose to partner with the Huck Institutes of the Life Sciences and an undergraduate student chapter of Material Advantage.