

EXECUTIVE SUMMARY

Center Vision and Organization

The underlying mission of the MIT MRSEC is to enable – through interdisciplinary fundamental research, innovative educational outreach programs, and directed knowledge transfer – the development and understanding of new materials, structures, and theories that can impact the current and future needs of society. The Center for Materials Science and Engineering (CMSE) seeks to bring together the large and diverse materials community at MIT in a manner that produces high impact science and engineering typically not realized through usual modes of operation. CMSE also fosters collaborative research with industry, government laboratories, and other universities, both national and international. Students and post-doctoral associates are trained in a highly interdisciplinary environment involving mentoring by multiple faculty members from different disciplines and departments.

Research Programs:

The MIT MRSEC encourages collaborative research through several mechanisms: interdisciplinary research groups (IRGs), seed and initiative projects, shared experimental facilities (SEFs), and outreach programs. Currently three IRGs, two initiatives, and five seed projects involving 31 faculty principal investigators are receiving support.

IRG-I: Design of Nanomaterials for Electrochemical Energy Storage and Conversion (Shao-Horn and Ceder co-leaders). This IRG seeks to accurately model, predict, and determine how thermodynamics, phase behavior, and kinetics are modified at the nanoscale, and use the resultant knowledge to design materials with energy and power-delivery capabilities far superior to those currently available.

IRG-II: Mechanomutable Heteronanomaterials (Ortiz and Cohen co-leaders). This IRG seeks to discover and develop new dynamically tunable multicomponent heterogeneous nanostructured systems with an emphasis on mechanical behavior, both theoretical and experimental. It is anticipated that the resultant materials, engineered to exhibit on-demand switchable mechanical properties, will impact a wide range of emerging biotechnologies.

IRG-III: Multimaterial Multifunctional Nano-Structured Fibers (Fink and Soljačić co-leaders). This IRG explores the design, fabrication, characterization, and physical phenomena of a new class of multicomponent nanoscale fiber materials containing conductors, semiconductors (glassy and crystalline) and insulators. These first of a kind integrated fiber devices have the potential to redefine completely the notion of functionally active fibers.

Initiative-I: Engineering Living Cells via Nanomaterials (Irvine and Rubner co-leaders). This initiative seeks to develop a fundamental understanding of how functionalized polymer multilayers and nanoparticles can be integrated with living cells in a manner that preserves cell viability and processes, and allows for new synthetically engineered functionality.

Initiative-II: New States of Frustrated and Correlated Materials (Lee and Nocera co-leaders). This initiative seeks to synthesize, characterize and examine the fundamental spin physics of new, single crystal materials based on a two-dimensional triangular and kagomé lattice.

Seed Projects: Nanoparticle Control/Transport using Mobile Magnetic Domain Wall Traps (G. Beach); Ultrafast Dynamics of Low Energy Excitations in Frustrated Materials (N. Gedik); Tailoring Optical Properties of Semiconductor Nanomaterials (S. Gradečak); Suspended Graphene Devices for Quantum Electronics and Nanosensing (P. Jarillo-Herrero); Large Area, Few-Layer Graphene Films for Various Applications (J. Kong).

Director's Overview

Diversity Plan: CMSE's diversity plan includes three key elements: 1) implementation of strategies to increase the diversity of participants in existing education programs; 2) development of new outreach programs that specifically target women and underrepresented minority groups; and 3) establishment of collaborations with MIT administration and departments that are working to address the diversity challenge in science and engineering.

Recent activities: To impact in a significant manner the diversity challenge, it is critical for CMSE faculty to be involved in institute-wide discussions and activities aimed at enhancing diversity at all levels within the institute. During this funding period, **Rubner** participated in a day-long Diversity Leadership Congress convened by MIT President Susan Hockfield. This conference brought together 320 academic, administrative and student leaders to focus on ways to promote diversity and inclusion across the Institute. CMSE is also fortunate to have two of CMSE faculty (**Ortiz** and **Hammond**) serving as members of an institute committee spearheading the Initiative for Investigation of Race Matters and Underrepresented Minority Faculty at MIT.

CMSE's Community College Program (CCP), a targeted REU program engaging participants from two local community colleges that enroll significant numbers of minority students, continues to have impact. Over the four-year history of the CCP, 76% of the participants have been minority students and 52% have been women. Of the participants who have completed their study at community college, at least 79% have enrolled in bachelor's programs. Recently this program was expanded to include day-long visits to CMSE by students from classes taught by community college partners.

In an emerging partnership with the Universidad Metropolitana (UMET) in San Juan, Puerto Rico, CMSE has launched a new pilot program aimed at students in economically challenged regions of Puerto Rico. Beginning this spring, UMET students will spend two weeks at MIT working with MIT graduate student mentors within CMSE SEFs on MRSEC research. In December, the UMET and MIT students will participate in a two-day symposium at UMET in which they will make presentations to pre-college students and teachers from local high schools. Aside from enhancing the students' presentation skills, the objective of this portion of the program is to broaden its impact and to help recruit young students into science and engineering.

Education Activities: CMSE educational outreach programs encompass a broad range of activities and age levels with participation from middle school students and teachers, undergraduates, and high-school students and teachers. A summary of programs planned for this coming year follows.

Undergraduate programs: Community College REU Program (4 summer research students, 20-40 students attending day-long events): This program targets community colleges in the greater Boston area with a significant enrollment of underrepresented students (40-55%). *Summer Research Internship Program (REU):* CMSE plans to support 11 undergraduates from institutions across the country in this tailored nine-week REU program. *Undergraduate Research Opportunities Program (UROP) (5-8 students):* The Center will provide opportunities for MIT undergraduates to participate in MRSEC research through MIT's UROP.

Teacher Programs: Research Experience for Teachers (RET) (8 teachers): CMSE will sponsor middle and high school science teachers in this two-tier RET program.

Science Teacher Enrichment Program (STEP) (5 teachers): This is a one-week engineering design workshop for middle and high school science teachers.

K-12 Student Programs: Women's Technology Program (WTP): CMSE will collaborate with the Department of Electrical Engineering and Computer Science to present this competitive four-week residential program to 40 high school women. CMSE will contribute to this goal by teaching a hands-on engineering design lab during four days of the program. *Science and Engineering Program for Middle School Students (24 students):* CMSE will offer this week-long, minority focused summer program to Cambridge middle school students. Graduate students, undergraduates and staff lead the students through a wide variety of hands-on and inquiry-based activities.

Additional Activities: MRSEC faculty and students will provide materials science content for special public events such as the MIT Museum's Family Adventures in Science and Technology and the third annual citywide Cambridge Science Festival (April 2009). These latter events are usually attended by hundreds of people from local communities.

Shared Experimental Facilities (SEFs): The SEFs (totaling 11,900 sq. ft. of space) represent a critically important component of the MRSEC and, indeed, the broader MIT research landscape. CMSE currently runs four major facilities: Materials Analysis, Crystal Growth and Preparation, Electron Microscopy, and X-Ray Diffraction. This past year, more than 900 individual users, from both inside and outside of MIT, utilized these facilities to conduct research, engage in educational outreach activities and teach MIT laboratory classes.

During this period, the process of equipping the JEOL 2011 TEM/STEM with a Gatan catholuminescence (CL) system was completed. The CL-STEM system enables characterization of nano-structured materials via electron excited optical transitions with spatial resolution that is unattainable with any other technique. In addition, after gathering extensive input from an ad-hoc committee comprising MIT faculty, and a complete review by the CMSE Internal Advisory Committee (IAC), a decision was made to purchase a dual-beam focused ion-beam milling system (FIB), which will be used for preparation of TEM specimens, for nano-lithography, and for serial sectioning and subsequent 3-D reconstruction of solid samples. Delivery of this new equipment is expected sometime this summer.

Industrial Outreach and Knowledge Transfer: To insure that important developments arising from MRSEC research are effectively transferred to colleagues in industry, CMSE works closely with MIT's Industrial Liaison Program (ILP) and Materials Processing Center (MPC). In collaboration with MPC, CMSE co-organized an annual industry-directed symposium entitled "Materials Day at MIT." The title of this year's event was "Nanostructure to Infrastructure to Sustainability." Guests attended the meeting from industry, government laboratories, hospitals, MIT, and other universities.

Three new start-up companies with connection to CMSE research have been launched. Kateeva was started by Prof. Vladimir Bulovic (supported by the previous MRSEC award) and several of his MRSEC-funded group members, along with MIT Prof. Martin Schmidt. The mission of Kateeva is to commercialize a new technology that could radically change the manufacturing paradigm for the flat panel display industry. WiTricity Corporation, on the other hand, was founded to commercialize a new technology for wireless electricity, pioneered by MIT Prof. Marin **Soljačić**. WiTricity can be used to provide direct wireless power for consumer electronics, industrial equipment, and existing electric transport vehicles. The newest CMSE-related start-up, Svaya Technologies, was founded by Prof. **Hammond** and colleagues in

September 2008. This Boston-area company will commercialize a new thin film manufacturing process that emerged, in part, from layer-by-layer research that was pioneered by an IRG funded during the previous MIT MRSEC grant (IRG-II).

Center Management: MRSEC activities are guided and supported by five committees, including a Science and Engineering External Advisory Board (SEEAB) composed of leaders of industrial and government laboratories and key faculty from academic institutions. Two members of the SEEAB stepped down this past year: Dr. Martin Blume, after many years of valuable service to CMSE, and Prof. Anna Balazs (U. of Pittsburgh), to avoid conflict of interest due to her recently activated collaboration with members of IRG-II. The CMSE director is currently soliciting/reviewing the names of qualified candidates and will reconstitute this board before the end of the year. During the Fall of 2008, CMSE conducted an institute-wide competition for new seed proposals. Fifteen proposals from six different MIT departments were received; of these, five new seeds were funded.

Key Accomplishments

Intellectual Merit: IRG-I members have leveraged earlier theoretical predictions by the group that suggested that extremely high lithium ion speeds are possible in lithium iron phosphate battery materials (LiFePO_4), to create batteries with amazing fast charging/discharging times. By changing the surface structure of this material, it was shown that it is possible to realize experimentally the predicted high power rates. Such high rate materials can be valuable in everything from rapidly charging cell phones to high-powered hybrid and plug-in hybrid vehicles. IRG-I research has also correlated the surface characteristics of Pt nanoparticles with the intrinsic activity for carbon monoxide and methanol electro-oxidation. This research suggests that increasing step densities on Pt nanoparticles can enhance specific activity up to 200%; translating to a reduction of Pt weight of up to 200% for a given fuel cell current output. Bio-derived gold nanowires of interest due to their potentially large electrocatalytic activity have been prepared from a genetically engineered virus with 2,700 copies of a specific gold binding sequence. This approach opens the door to the low temperature creation of nanostructured gold with tunable dimensions and properties.

IRG-II research has revealed through atomistic-based multiscale simulations that the concept of “mechanomutability” – i.e. the capability of a material to change its mechanical properties reversibly in response to an external stimulus, is indeed realizable. By using a model system of a surface-anchored array of carbon nanotubes, it was shown that, under the application of an external magnetic field, dramatic conformational changes occur that lead to variations in spatial patterning and a contact stiffness that can be changed reversibly from ~ 73 MPa to 910 MPa. Mechanomutable materials have many potential applications including control of cellular behavior, modulation of protein adsorption, the creation of nanoscale motors, tunable vibration absorption, and high spatial sensitivity variable sensors. Experimentally addressable mechanomutable materials have been created by using a templated layer-by-layer assembly approach. The resultant surface array of polymer nanotubes was found to exhibit a reversible pH-controlled swelling transition that produced significant changes in the shape, size and physical properties of the nanotubes.

IRG-III researchers demonstrated a new phenomenon in which a semiconductor cylindrical shell (inside of a fiber preform) undergoes a scaling process and evolves into an array of filaments during the fiber drawing process. This approach will enable, for the first time, the creation of fibers with a high density of electrical interconnects that may be potentially useful in enabling diverse large-area applications including energy related technologies such as photovoltaics and

thermoelectrics. Spontaneous cascaded Raman amplification was also demonstrated by this group as a practical and efficient means of power transfer from telecommunications wavelengths to mid-IR wavelength bands through use of conventional silica fibers and amplifiers. The fundamental mathematical basis for single-polarization polarization-maintaining fibers, was also identified, potentially leading to new classes of photonic-crystal fibers that operate in a single-polarization regime.

Initiative-I researchers have developed a number of new processes for attaching nanoscale elements onto living immune system cells. In one case, nanoscale thickness polymer backpacks that can be loaded with a wide range of functional materials including cancer drugs, imaging molecules and magnetic nanoparticles have been attached to living B-cells, T-cells and phagocyte cells. After attachment, all cell types were found to remain viable and, since only a portion of their cell surface has been occluded by the backpack, were able to carry out their normal functions such as cell migration. In the second case, 'lipid-enveloped' biodegradable polymer nanoparticles with the ability to encapsulate drug molecules in their core and/or incorporate drugs in the surface lipid bilayer, were attached to living T-cells by a directed thiol reaction scheme and were not endocytosed but remained on the cell surface. Although still in the early stages of development, these experimental findings in total suggest the exciting possibility of having immune system cells selectively target, carry and deliver therapeutic drugs to disease sites.

Initiative-II members, along with collaborators at Brookhaven National Laboratory and Nagoya University in Japan, have developed a new methodology for probing electronic properties at the atomic scale. This new approach allows one the ability to measure with atomic precision electronic properties generally thought of as "bulk" such as the "Fermi surface" – related to electron density. It is anticipated that this work will reveal a new understanding of correlated electron systems. This group also found that an organic-inorganic hybrid composed of spin-1/2 Cu ions on a structural perfect kagomé lattice, shows the absence of a spin-gap or magnetic ordering down to low temperatures. However, inelastic neutron scattering measurements revealed a new twist, below $T = 2$ K, a spin excitation appears which has a characteristic energy scale of about 0.6 meV. This feature is novel, and an explanation of its origins requires additional theoretical insight as well as further experimental investigations.

Broader Impact: A key objective of CMSE is to facilitate interdisciplinary research and education with the goal of yielding high impact activities in the multifaceted area of materials science and engineering. The Center works closely with MIT departments to recruit and develop new talent with expertise in areas that support the CMSE long-term mission. Close synergistic coupling to organizations at MIT charged with the mission of engaging industry in MIT research insures effective knowledge transfer and valuable industrial input and guidance. The educational outreach programs target often overlooked groups such as community college students at institutions with limited resources. The research programs and SEFs contribute to the education and training of numerous undergraduate and graduate students, postdocs, and high school and middle school teachers and students, as well as visitors from many companies and local universities. The diversity enhancement activities encourage a wide cross-section of people of all ages to participate in and pursue the science and engineering enterprise.

Long-Range Plans/Issues: Dr. Tony Garratt-Reed, a 35-year MIT employee and long-time SEF Technical Manager and electron microscopist in the EM SEF, retired in September of 2008. An extensive national and international search resulted in the hiring of Dr. Shiahn Chen, formerly an electron microscopist at the University of Maine at Orono.

CENTER STRATEGIC PLAN

Overall Mission: MIT has an exceptionally strong and broad effort in materials science and engineering. CMSE, an interdisciplinary center at MIT, plays the critical role of bringing this diverse materials community together by encouraging and supporting collaborative research and innovative educational outreach programs. The clear and important mission of CMSE is to encourage fundamental research and education in the science and engineering of materials for long-range applications that will address the current and future needs of society. To accomplish this mission, CMSE enables collaborative interdisciplinary research among MIT faculty and between MIT faculty and the researchers of other universities, industry and government laboratories. Industrial and educational outreach efforts are fully integrated into all center activities. CMSE reports directly to the vice president for research. This insures that CMSE can effectively promote collaboration between researchers at MIT from both the Schools of Engineering and Science. Hence, CMSE is in a unique position to encourage faculty from different departments and schools to work together on new problems that require an interdisciplinary approach. Four internal and one external committee provide guidance and input to the director and monitor all critical aspects of center activities.

Research: CMSE's research goal is to encourage collaborative research through several mechanisms: interdisciplinary research groups (IRGs), seed and initiative projects, shared experimental facilities (SEFs), and outreach programs. To insure that our research programs deliver the highest possible scientific and technological impact, we utilize an extensive review process involving internal and external evaluation of our programs. To become and remain a CMSE-supported researcher, it is necessary to successfully navigate this highly competitive, MIT-wide process. Regular meetings of our internal advisory board (IAC) insure that IRG leaders and our faculty educational outreach and SEF leaders understand and share a common vision for the center. Our Science and Engineering External Advisory Board (SEEAB) provides an outside perspective on the impact of our activities. This committee is composed of leaders of industrial, academic and government laboratories that support major efforts in long-range materials research and engineering. Important metrics utilized to evaluate our research programs include, for example, number, quality and impact of peer-reviewed publications, level and effectiveness of multi-investigator collaborative activities, engagement of graduate and undergraduate students in research, number of patents and licenses granted and effectiveness of knowledge transfer and outreach activities.

Education: CMSE offers a wide variety of educational outreach programs including programs directed at middle and high school students, K-12 teachers, women and minorities, undergraduates, and graduate students. The center's educational goal is to provide a portfolio of effective and innovative educational outreach programs that are integrated into our research activities and benefit from wide participation of MIT faculty and students. In all of our programs, specific measures are in place to promote and enhance diversity within each participant pool. CMSE's education committee consults on the direction of the education programs and facilitates the coordination of our programs with other outreach programs on campus. Assessment of our educational outreach programs against their objectives is accomplished by carefully crafted entrance and exit surveys and, where possible, by tracking of participant activities after completion of our programs. Another important metric is the level of subsequent involvement/collaborative interactions participants have with our center. We view our educational outreach activities as a vehicle for creating long-term relationships with, for example, local K-12 teachers and work to facilitate this process. To date, hundreds of students and teachers have taken advantage of the many resources available through our center.

Diversity: CMSE has a history of encouraging traditionally underrepresented minority groups and women to participate in materials research and education through its educational outreach programs, dedicated sponsorship of graduate research assistants, and efforts to coordinate

CMSE activities with other MIT programs. CMSE's diversity goals include three key elements: 1) implementation of strategies to increase the diversity of participants in our existing education programs; 2) development of new outreach programs that specifically target underrepresented minority groups; and 3) initiation and execution of collaborations with other units at MIT that are working to address the diversity challenge in science and engineering. One key metric for assessing the impact of these activities is the number of women and minorities participating in our programs. However, it is not sufficient to simply increase numbers. We recognize that it is extremely important to provide an experience to our participants that is tailored and sensitive to their specific needs. Thus, an important goal is to establish a support infrastructure that insures that our program objectives are realized. As an example, in our community college program, we work closely with a faculty member from each college to monitor the progress of participants and better understand their needs. Close relationships of this type also help us track the subsequent progress of participants.

Shared Experimental Facilities: A key objective in this case is to establish state-of-the-art facilities that provide and maintain critically enabling instrumentation for our MRSEC investigators and, at the same time, serve as an important resource to the broader MIT materials community and beyond. An additional goal is to minimize the cost to users to make available an important educational training opportunity to all interested outreach participants, students and post-doctoral associates. To accomplish these important goals, we have assembled a highly motivated and engaged professional support staff and a substantial support infrastructure. Over the past five years or so, our user base has steadily increased from about 500 to 900 individual users. Long-term issues include the rising costs of modern instrumentation and service contracts. To address this important problem, we aggressively seek cost-sharing opportunities with other laboratories, departments and centers at MIT. This has allowed us to purchase, for example, expensive electron microscopes that vastly exceed our equipment budget. Faculty-based user groups are utilized as needed to provide input on facilities performance and, in conjunction with our IAC, to make recommendations for new equipment purchases. To insure compliance with our long-term mission, the assistant director of our center manages directly all important aspects of the facilities.

Knowledge Transfer: MIT has a long-standing history of promoting collaboration with, and knowledge transfer to, industry. To facilitate the transfer of the fundamental knowledge generated within our program to the outside world, CMSE works effectively with MIT's Materials Processing Center (MPC) and Industrial Liaison Program (ILP). Our goal is to keep industry, government laboratories and other universities aware of the latest developments and discoveries from within our center and, where possible, facilitate technological developments that will impact society and the economy. This goal is accomplished through participation in MPC and ILP organized outreach events such as "Materials Day at MIT" and through numerous ILP arranged meetings at companies and with company researchers and technical managers. Start-up companies based on CMSE research are another important vehicle for knowledge transfer.