Report of the MPSAC Subcommittee on the American Competitiveness Initiative
May 3, 2007

I. Background

The Augustine report,[1] "Rising Above the Gathering Storm" included the following overarching recommendation:

> *Sustain and strengthen the nation's traditional commitment to long-term basic research that has the potential to be transformational to maintain the flow of ideas that fuel the economy, provide security, and enhance the quality of life.*

The report further recommended an increase of 10% per year for 7 years in the nation's investment in long-term basic research in physical sciences, engineering, mathematics, and information sciences. MPS, in conjunction with its collaborative partners in ENG, CISE, OCI and ERE, is ideally situated to have a dramatic impact on achieving the goals of ACI as well as the Innovation Agenda already circulating in Congress. Both short-term and long-term planning is required to provide guidance to the directorate regarding areas for future investment. There is a strong sense that economic competitiveness comes from fundamentally new innovations, not from incremental improvement of existing technology. ***Truly transformational outcomes will result only from increased and sustained investment in basic physical sciences, mathematics and related fields.***

The subcommittee was charged with reviewing past investments as well as recommending future areas of interest. The committee met by teleconference on 3/1/07, 3/14/07, 3/29/07 and 4/24/07 to review the FY 2008 budget request and to suggest areas for increased visibility.

II. Review of the FY 2008 budget request vis-à-vis ACI

A large fraction of the FY 2008 budget request could be aligned with ACI, particularly in the areas of ***Science Beyond Moore's Law***, which was a major feature in several divisions' requests. These and others are further articulated below:

• In AST, funding that enhances cyberscience and cyberinfrastructure including the development of tools to manipulate and analyze large and heterogeneous data sets represents a major alignment with ACI. AST facilities, such as the Atacama Large Millimeter Array that is currently under construction, exemplify the unique, technologically advanced, large-scale "tools of science" that ACI calls out as essential to maintaining US leadership in the global economy.

• In CHE, nearly all areas of the portfolio can be viewed as aligned with ACI: nanoscience, complexity and the molecular basis of life processes facilitate the discovery of new materials as well as new molecular processes that support both nanotechnology and the pharmaceutical industry; science beyond Moore's law is aimed at discovery of single-molecule electronic devices and self-assembling schemes to facilitate the electronics industry; sustainability issues address the growing needs of the US chemical, energy and agricultural industries to utilize natural resources in an

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[1] *Rising Above The Gathering Storm: Energizing and Employing America for a Brighter Economic Future,* Natl. Acad. Press, 2007.

environmentally sound fashion; cyber-enabled discovery is aimed at computational modeling of molecular processes that have ramifications in remote sensing or characterization of reactive species.

• In DMR, all areas of experimental and theoretical research have a bearing on ACI including condensed matter physics, solid-state chemistry and polymers, biomaterials, structural and high temperature metals and ceramics, nano-scale material systems, electronic, magnetic and photonic materials. New materials are critical to the ACI issues of energy, sustainability and feedstock for manufacturing. Basic advances in our understanding at the atomistic level of fundamental reactions and interactions and how they control properties will open new avenues for designing and synthesizing novel complex materials with unique and adaptive properties.

• In DMS, the area of science beyond Moore's law is clearly aligned with ACI, and DMS can provide fundamental advances in algorithm design, scalability, and quantification of errors and uncertainty. Through fundamental research, DMS strengthens the core of many disciplines that apply mathematics and statistics, and like AST, contributes to the analysis and understanding of large data sets.

• In PHY, the ability to generate predetermined quantum states in atoms and molecules provides the underpinnings for a quantum-level technology that offers a revolutionary approach to the tools of computation and communication. Analytical and computational techniques needed for extraction of information from large data sets generated in experiments in elementary particle physics lead to new approaches for massive signal processing. Distribution of the data to the worldwide physics community fosters approaches such as grid computing. The advances in biological physics are aligned to the ACI's goals of developing the healthcare industry. Advances in accelerator technology also impact healthcare.

All of the divisions contribute in a major way to the training of a diverse and highly skilled technical workforce. The vast majority of the MPS budget is used to train students and provide advanced instrumentation for use by these students who will go on to be the nation's next generation of innovators. *This is of paramount importance to the ACI and should continue to be emphasized.*

III. Areas for continued/increased visibility in the FY 2009 budget

A December 2006 NSF workshop entitled "Sustaining America's Competitive Edge" outlined seven priority areas of special opportunity in science and engineering:

- Plant Science: from biofuels to nutrition
- Complex Structural Materials Systems: high performance materials for construction
- Electronic and Optical Materials and Systems: theory and design of new materials for communications and information technology
- Energy and Materials: photovoltaics, hydrogen generation, transport and storage, advanced nuclear technologies, advanced coal technologies, batteries, etc.
- Nanotechnology--Science and Applications: molecular assemblies
- Development of New Pharmaceuticals: from synthetic chemistry to biophysics
- Imaging Science and Technology: medical diagnostics, *in situ* techniques for dynamic studies of reactions and interactions, and remote sensing

All of the above areas can be enhanced by basic research activities in the MPS domain.

Furthermore, they represent the largest sectors of our technology-based economy—energy, electronics, and pharmaceuticals—and so the long-term effects of fundamental research and innovation will be dramatic.

In the coming year, ***Sustainable Energy*** is thought to be an over-arching concern whose solutions can be addressed through investment in basic research. Meeting future demands for energy without overtaxing the environment is an enormous challenge that cannot be addressed by any single technology, or by any single funding agency. Interim solutions may rely on more efficient use of coal, ethanol and biofeedstocks, but long-term solutions that do not generate CO_2 must be sought now. Nine long-term challenges that are outlined in a recent *Science* perspective by Whitesides and Crabtree[2] are:

- The oxygen electrode problem: fuel cells and the production of H_2
- Catalysis by design: processes in the production and storage of energy
- Transport of charge and excitation: making cost-effective solar cells
- Chemistry of CO_2: large-scale physical and chemical properties of CO_2 in the environment
- Improving on photosynthesis: uptake and processing of CO_2 and other light-mediated fixation reactions
- Complex systems: understanding multi-component systems with non-linear interactions; emergent behavior
- Efficiency of energy use: new strategies for reducing wasted energy
- Chemistry of small molecules: H_2O, H_2, O_2, CO_2, CO, NO_x, O_3, NH_3, SO_2, CH_4, CH_3OH, HCl
- New ideas: growing the Earth's biomass, stimulating photosynthesis in the oceans, new nuclear power cycles, room-temperature superconductivity, biological production of H_2, new concepts in batteries, etc.

NSF and DOE must act synergistically as they do in other areas, and, for example, as NSF and NASA do in the field of astronomy. NSF should focus on long-term fundamental research from which transformational science will emerge providing entirely new strategies to attack sustainable energy problems. Partnerships between NSF and DOE might occur at the divisional level among specific programs that derive added benefit from such a joint approach.

The committee had the following recommendations for additional emphasis in 2009 beyond those just described.

- Increased emphasis of cyber-enabled research for handling and extracting knowledge from large and heterogeneous data sets, for assimilating observational and experimental data into computational models, for creating virtual environments that allow humans to interact with data and models, and for underlying advances in imaging and signal processing, including multi-modal and real-time aspects. While CISE contributes to the implementation of these aspects of cyberinfrastructure, MPS is a major driver and algorithmic enabler.
- Development of new algorithms and computational methods to model multiscale, non-equilibrium systems, and to understand interacting complex systems and emergent phenomena.
- Discovery of new molecular materials and science "Beyond the Molecule" to

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[2] Whitesides, G. M.; Crabtree, G. W. *Science* **2007**, *315*, 796.

help understand complex phenomena. Additional support for the discovery of new reactions and new assemblies would impact health sciences and the pharmaceutical industry as well as materials science and technology. "Responsible chemistry" aimed at minimizing the impact on the global environment is a key aspect of this research.

- Photochemistry and photophysics aimed at understanding photodynamic processes and designing advanced photonic materials. These areas specifically impact energy and electronics.
- The biological interface with mathematical and physical sciences including chemistry and physics of the brain, synthetic and computational mimicry of biological processes, biomolecular machines, and the human impact on the environment.
- Quantum computing, molecular electronics, and science "beyond Moore's law" should continue to be a driver for the development of quantum-based technology, an approach that uses the quantum behavior of individual quantum states, e.g. of molecules or spins, as the basis for information storage and manipulation.
- New materials for applications in extreme environments characterized by high temperature, high pressure, stress, corrosion, oxidation, or intense irradiation. These span needs in the nuclear, coal, gas, and photovoltaic energy generating systems as well as hydrogen production facilities. The operational environments envisioned for advanced energy technologies place stringent demands on materials, and to meet the challenge, new strategies for designing, producing and assessing properties of materials systems are needed. This requires discovery of the fundamental atomistic processes, reactions and interactions operating in these environments and of how they dictate macroscopic properties.

IV. Development of a technical workforce skilled in physical sciences and mathematics.

Regarding the workforce, MPS should continue to provide leadership in expanding and diversifying the scientific workforce. Given national trends of diminished interest and lower achievement in science and math among school children, especially minorities, major initiatives should be launched to achieve a "Sputnik-like" call to action bringing the best young minds to science. For example, the I2U2 program that utilizes GRID technology to involve K12 students and teachers with physical science in large-scale projects goes beyond any one small experiment to create a national and international network.

With foreign enrollments declining at US institutions, the technical workforce should be increased domestically, particularly through outreach programs to underrepresented populations.[3] In addition, mechanisms to retain the best foreign students in the US would be desirable since many US-trained Asian students are now being courted back to their countries of origin due to rapidly rising investments in science and technology in

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[3] *Land of Plenty: Sustaining America's Competitive Edge in Science, Engineering and Technology.* A Report of the Congressional Commission on the Advancement of Women and Minorities in Science, Engineering and Technology Development, September 2000. http://www.nsf.gov/pubs/2000/cawmset0409/cawmset_0409.pdf

China and India.[4] Current US immigration policies pose very substantial barriers for foreign students wishing to launch their scientific careers in the US.

The February 2001 Hart-Rudman report on National Security/21st Century listed as their second key recommendation for change, *"revitalizing America's strengths in science and education,"* including a doubling of the science budget by 2010. MPSAC responded in May 2002 by suggesting that NSF should expand its role as the steward of US science research capabilities, and toward that end, a number of cross-disciplinary workshops were organized evaluating the state of the art of various scientific frontiers. In addition, MPSAC suggested that the Directorate should take a leadership role in coordinating efforts with other funding agencies. Ongoing educational efforts such as REU, RET, IGERT and VIGRE programs were also highlighted in that report.

MPS science areas are often showcased in the media and can be effective in recruiting the most brilliant and ambitious young minds into science and technology fields. Combining accessible narratives with captivating imagery from cosmic to nano-scales, researchers from MPS will continue to capture the imagination and convey the excitement of technology-enabled research at the frontiers of knowledge and innovation. These efforts should be enhanced to strengthen the pipeline of students entering scientific disciplines.

V. Past investments that can be articulated in terms of ACI

Reviewing the MPS web pages indicates that the Directorate has effectively been supporting ACI-related physical sciences and mathematics for a number of years. Many examples are highlighted at:

- Astronomy: http://www.nsf.gov/news/index.jsp?prio_area=2
- Chemistry and Materials: http://www.nsf.gov/news/index.jsp?prio_area=4
- Mathematics: http://www.nsf.gov/news/index.jsp?prio_area=9
- Physics: http://www.nsf.gov/news/index.jsp?prio_area=11

The subcommittee recognizes that the Division Directors are well poised to distill from their individual portfolios the past investments that best represent ACI-aligned outcomes, and it recommends that the Directorate continue to seek this valuable input from them. Publicity concerning MPS-funded science and mathematics educates the public, guides teachers and researchers, informs legislators, and improves the image of scientists, thereby attracting new students for the as yet unimagined science careers of the future.

VI. Mechanisms of enhancing the MPS investment for competitiveness and innovation.

MPS funding aligned with ACI can take many forms in terms of the types of grants awarded. In order to attract and retain some of the nation's best scientists, awards to individual "ACI Fellows" would be effective. As the problems tackled become more complex and interdisciplinary, additional funding for centers and collaborative research projects will be necessary. Advanced instrumentation, facilities and cyberinfrastructure

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[4] For information concerning the decline of the workforce in Chemistry, see the recent Casey report: *The Future of US Chemistry Research: Benchmarks and Challenges,* National Research Council, 2007. ISBN: 978-0-309-10533-0

will be required to keep US science and mathematics researchers and educators competitive in their work. Importantly, these enhancements should not erode the individual investigator awards in core disciplines since these are the incubators of new knowledge and innovation.

MPS has a strong tradition of fostering innovative ideas in education that help diversify the workforce and expand the participation of underrepresented groups in science and engineering. New and continuing funding mechanisms should guide researchers toward best practices in broadening participation.

VII. Summary

Advances in economic competitiveness stem from fundamentally new innovations, not from incremental improvements in existing technology. Transformational outcomes must be seeded by increased and sustained investment in basic physical sciences and mathematics.

The subcommittee identified many components of the FY 2008 budget request that, in alignment with ACI, would promote the major sectors of our economy, including energy, health, and electronics. Briefly, these include science beyond Moore's Law, cyberscience and the analysis of large data sets, the molecular basis of life processes, new synthetic methods and advanced materials with tailored or functional properties.

Areas for continued and increased visibility in the FY 2009 budget request include all of the above with additional emphasis on sustainable energy and the global environment, science "beyond the molecule", cyber-enabled research, new algorithms and computational methods, quantum computing and molecular electronics (including advances beyond Moore's Law), photochemistry and photophysics, advanced material systems and the biological interface with physical sciences and mathematics.

Critical to America's competitiveness is the education of the next generation of innovators supported by an expanded technological workforce. MPS should continue to provide leadership in science and math education, teacher training and outreach activities, and the provision of tools that support the nation's science education efforts. Captivating, recruiting, and retaining the nation's best young minds in physical and mathematical sciences should be given very high priority.

The subcommittee recommends that division directors continue to bring forward their best examples of ACI-related outcomes from their portfolios in order to inform and stimulate a scientifically-minded public.

Mechanisms must be found to spur new collaborations, to recruit and retain the best scientists working in innovative areas, and to broaden participation in physical sciences and mathematics while fostering the core disciplines.

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