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Key Findings and Recommendations: Frontiers of Materials Research – A Decadal Survey

Key Finding	Key Recommendation(s)
Advanced materials are increasingly central to everyday life and well-being. New developments are products of the broad and interdisciplinary field of materials science, drawing on all the traditional fields of science, engineering, and more recently, computer and data science (algorithms, big data, artificial intelligence, machine learning), with the special perspective that comes from a focus on materials. The health and future growth of materials research, and its capability to serve society, depend critically on the flow of information among its stakeholders, from university researchers to industrial engineers to government labs.	*Government agencies, led by the OSTP, should work with high priority to foster communication among materials research stakeholders through the support of interdisciplinary research and the development of modalities for freer flowing interactions among universities, private enterprise (including start-up ventures), and national laboratories.
Many of the real-world challenges and opportunities in materials research occur at the intersections among traditional disciplines, and at the interfaces between fundamental and applied research. Pure science is stimulated by proximity to applied research. Collaboration and information transfer among different disciplines and among academia, industry, and government laboratories greatly increases the likelihood of successfully meeting these challenges and capitalizing on these opportunities.	*Government agencies, led by the OSTP, should work with high priority to foster communication among materials research stakeholders through the support of interdisciplinary research and the development of modalities for freer flowing interactions among universities, private enterprise (including start-up ventures), and national laboratories. The White House OSTP should provide leadership in the development of awards that enable diverse funding agencies to work together when needed to facilitate collaboration among university and industry researchers. The NSF should develop a new type of center that will enable, and indeed stimulate, students, faculty, and industrial scientists and engineers to work side by side. Such a Discovery to Translation Materials Research Center (DTMRC) would create a unique learning and research environment. The effort should be supported by several NSF directorates and should continue for a minimum of a decade.
The integrated computational materials science and materials engineering methodology has had a	All government agencies funding materials research should encourage the use, when appropriate, of

significant impact on product development in specific industries, as the committee has learned through industrial input. There is potential for further impact through the inclusion of integrated data sciences into the materials research for all length scales and material types.	computational methods, data analytics, machine learning, and deep learning in the research they fund. They should also encourage universities to provide students of science and engineering exposure to these new methods by 2022.
Basic research in fundamental science directions, meaning work that neither anticipates nor seeks a specific outcome, is the deep well that both satisfies our need to understand our universe and feeds the technological advances that drive the modern world. It lays the groundwork for future advances in materials science as in other fields of science and technology. Discoveries without immediate obvious application often represent great technical challenges for further development (e.g., high-Tc superconductivity, carbon nanotubes) but can also lead to very important advances, often years in the future.	It is critically important that fundamental research remains a central component of the funding portfolio of government agencies that support materials research. Paradigm-changing advances often come from unexpected lines of work.
The Materials Genome Initiative, and the earlier Integrated Computational Materials Engineering approach, recognized the potential of integrating and coordinating computational methods, informatics, materials characterization, and synthesis and processing methods to accelerate the discovery and deployment of designer materials in products. The translation of these methodologies to specific industries has resulted in numerous successful applications that have reduced the development time with corresponding cost savings.	The U.S. government, with NSF, DOD, and DOE coordinating, should support the quest to develop new computational and advanced data-analytic methods, invent new experimental tools to improve the properties of materials, and design novel synthesis and processing methods. The effort should be accelerated from today's levels through judicious agency investments and continue over the next decade in order to sustain U.S. competitiveness.
Research into metals, alloys, and ceramics continues to provide fundamental understanding of atomic-scale processes that govern synthesis-microstructure-property relations in many classes of materials. Armed with this understanding and state-of-the-art synthesis, characterization, and computational tools, novel alloys and micro/nanostructures with extraordinary properties are being realized. Traditional areas of materials research can have surprising new developments, for example, in multicomponent, high-entropy alloys and inorganic glasses.	Federal funding agencies (NSF, DOE, DOD) should maintain robust programs to support, and in some cases, expand fundamental research in long-established areas such as metals, alloys, and ceramics.
Quantum materials science and engineering, which can include superconductors, semiconductors, magnets, and two-dimensional and topological materials, represents a vibrant area of fundamental research. New understanding and advances in materials science hold the promise of enabling transformational future applications in computing, data storage, communications, sensing, and other emerging areas of technology. This includes new computing directions outside Moore's law, such as quantum computing and neuromorphic computing, critical for low-energy alternatives to traditional	Significant investments by, and partnerships among, NSF, DOE, NIST, DOD, and IARPA will accelerate progress in quantum materials science and engineering, so crucial to the future economy and homeland security. U.S. agencies with a stake in advanced computing, under the possible leadership of DOE's Office of Science and NNSA laboratories and the DOD research laboratories (ARL, NRL, AFRL), should undertake to support new initiatives to study the basic materials science of new computing paradigms during the next decade. To remain internationally competitive, the U.S. materials research community must continue to grow and expand in these areas.

processors. Two of the National Science Foundation (NSF)'s "10 big ideas" specifically identify support of quantum materials (see *The Quantum Leap: Leading the Next Quantum Revolution* and *Midscale Research Infrastructure*).	
Materials science and technology has an enormous impact on the quality and sustainability of Earth's environment across the entire spectrum of materials types. This is another important opportunity for university, national laboratory, and industry cooperation.	Research in numerous directions that improve sustainable manufacturing of materials, including choices of feedstocks, energy efficiency, recyclability, and more, is urgently needed. Creative approaches for funding materials research toward sustainability goals should be developed by NSF, DOE, and other agencies.
Progress in three-dimensional (3D) characterization, computational materials science, and advanced manufacturing and processing have enabled an increasing digitization across disciplines of materials research and has in some cases dramatically accelerated and compressed the time from discovery to inclusion in new products.	Federal agencies (including NSF and DOE) with missions aligned with the advancement of additive manufacturing and other modes of digitally controlled manufacturing should by 2020 expand investments in materials research for automated materials manufacturing. The increased investments should be across the multiple disciplines that support automated materials synthesis and manufacturing. These range from the most fundamental research to product realization, including experimental and modeling capabilities enabled by advances in computing, to achieve the aim that by 2030 the United States is the leader in the field.
Infrastructure at all levels, from midscale instrumentation for materials characterization, synthesis, and processing with purchase costs of \$4 million to \$100 million in universities and national laboratories to large-scale research centers like synchrotron light sources, free electron lasers, neutron scattering sources, high field magnets, and superconductors is essential for the health of the U.S. materials science enterprise. Midscale infrastructure, in particular, has been sorely neglected in recent years, and the cost of maintenance and dedicated technical staff has increased enormously.	All U.S. government agencies with interests in materials research should implement a national strategy to ensure that university research groups and national laboratories have local access to develop, and continuing support for use of, state-of-the-art midscale instruments and laboratory infrastructure essential for the advancement of materials research. This infrastructure includes materials growth and synthesis facilities, helium liquefiers and recovery systems, cryogen-free cooling systems, and advanced measurement instruments. The agencies should also continue support of large facilities such as those at Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, Argonne National Laboratory, SLAC National Accelerator Laboratory, National Synchrotron Light Source II (Brookhaven National Laboratory), and National Institute of Standards and Technology—and engage and invest in long-range planning for upgrades and replacements for existing facilities.
Intense competition among developed and developing nations for leadership in the modern economic drivers, including smart manufacturing and materials science, will grow over the coming decade.	The U.S. government, with input from all agencies supporting materials research, should take coordinated steps beginning in 2020 to fully assess the threat of increased worldwide competition to its leadership in materials science and in advanced and smart manufacturing. The assessment program, which should be established on a permanent basis, should also define a strategy by 2022 to combat this threat.

The key findings and recommendations found in the above table spanned four chapters. The first four came from Chapter 1. Brief Survey of Developments over the Decade; the next four came from Chapter 3. Materials Research Opportunities; the next two came from Chapter 4. Research Tools, Methods, Infrastructure, and Facilities; and the last one came from Chapter 5. National Competitiveness. In addition to the key findings and recommendations, the report also enumerated an additional twenty-four findings and associated recommendations across chapters 3, 4, and 5. One key recommendation regarding the importance of intergovernmental and broader materials stakeholder communication was reiterated twice and is noted with an asterisk (*) in the table.

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