# A Material World



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#### BENEFIT OF MATERIALS TO SOCIETY

Two key goals in the field of materials research are to discover new materials and gain an improved understanding of materials and phenomena. Often the focus is placed on elucidating the relationships between processing, structure, and properties to enable the creation of better and more functional materials. Discoveries and advancements reflect the breadth of practitioners. Material researchers draw from a medley of backgrounds - with expertise in e.g., biology, chemistry, engineering, geology, manufacturing, mathematics and physics. From this foundation, they explore the quantum and classical worlds at length scales ranging from the atomic and molecular to the macro in the pursuit of new knowledge about our solid-state world. The next new communication device (cell phone, television, personal fitness monitor), automobile (electric and hybrid vehicles), and key transportation structure (such as roads and bridges) we rely on everyday exists because of advances in materials. Materials have played a central role in human societal progress as far back as the Stone Age, when humankind began to use tools, and fast forwarding to the Silicon Age with the invention of the transistor and modern-day electronics. Let's face it, we live in a "material world" and increasingly, as society's needs become more complex, so do the demands on materials researchers.

Today, material researchers have a higher responsibility to help the world meet the challenges facing society. Although materials research has expanded to include several disciplines and is inherently "interdisciplinary", this is not enough. The requirements have (once again) increased due to the growing complexity of societal problems and their solutions. Materials researchers are now challenged to change their modes of operating to have cyclic synergism ("closing the loop") with systems-level thinking (alongside the required deep exploration and understanding of details into fundamental mechanisms). Also, the field of materials research needs to further expand to embrace data and manufacturing scientists and to more fully engage environmental, social, and economic sciences.

#### **CURRENT SOCIETAL CHALLENGES**

First, looking back, the National Academy of Engineering defined the greatest accomplishments of the twentieth century<sup>1</sup> where materials are the key to many of them.<sup>2</sup> It follows that materials will be critical to solving many of the world's grand challenges in the twenty-first century (Table I)<sup>3</sup> and to securing a higher standard of living.

The U.S. federal government, and specifically, the National Science Foundation (NSF), are undertaking dedicated efforts on several fronts to rise to these challenges. We contend that it is essential to examine sustainability (life cycle, preservation and stretching of resources), have resilience and adaptability (to deal with the unexpected and evolve), advance manufacturing (for safety, efficiency and state-of-the-art), and improve quality of life (through better health and optimization of time).

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# Sustainability

Sustainability of our environment and resources is the key to our future, and a responsibility in the domain of scientists. Sustainability has garnered attention at the highest levels including The White House. They have examined this issue from several angles; we provide just a few examples below:

- · Combating Climate Change (Clean Power Plan)<sup>4</sup>
- Building a Sustainable Water Future<sup>5</sup>
- Sustainable Farming for Global and National Food Security<sup>6</sup>
- Educating the Next Generation of Environmental Stewards<sup>7</sup>

The Materials Research Society (MRS) published a special issue of the MRS Bulletin: Materials for Sustainable Development, identifying challenges in manufacturing, transportation, infrastructure, energy, water and teaching.8 In his introductory article, Green notes: "Every human endeavor is affected by the ramifications of sustainable development because none of our material resources are infinite... sustainable development is a huge field that captures the concepts of environmental stewardship, materials management, green manufacturing, renewable and clean energy technologies, and water and air management under one tent." In 2010, NSF began in earnest to address these issues through a new initiative, Science, Engineering and Education for Sustainability (SEES).9 The stated mission of SEES is to advance science, engineering, and education to inform the societal actions needed for environmental and economic sustainability and sustainable human well-being.<sup>10</sup> The materials research community is responding to the challenge in a myriad of ways. Accordingly, NSF investments have been made across a range of materials that serve as components in many system solutions, particularly in the energy sector. Improving properties, expanding operational temperature ranges and using safe and abundant elements are also key.

Table I. NAE grand challenges (http://www.engineeringchallenges.org/challenges.aspx)

TECHNOLOGY	ENERGY	ENVIRONMENT	HEALTH
Secure cyberspace. Enhance virtual reality. Advance personalized learning. Engineer the tools for scientific discovery. Prevent nuclear terror.	Make solar energy affordable. Provide energy from fusion.	Develop carbon sequestration methods.  Manage the nitrogen cycle.  Provide access to clean water.  Restore and improve urban infrastructure.	Advance health informatics. Engineer better medicines. Reverse-engineer the brain.



Fig 1. Dr. Carley Corrado, Director of Business Development at Soliculture.

NSF created a new cross-directorate opportunity, Sustainable Chemistry, Engineering, and Materials (SusChEM), within the SEES portfolio in 2012.11 This notice about proposal submissions challenges science and engineering researchers to consider sustainability principles in their fundamental research endeavors.12 Simultaneously, NSF launched a short-term SEES Fellows program,13 which sought to "advance science, engineering, and education to inform the societal actions needed for environmental and economic sustainability and human well-being while creating the

necessary workforce to address these challenges." One SEES Fellow awardee, Dr. Carley Corrado took on the challenge to extend her expertise (beyond Physical Chemistry) and apply sustainability principles to her fundamental research (Fig. 1). As a post-doctoral fellow, she joined the physics laboratory of Prof. Sue A. Carter at the University of California, Santa Cruz where they worked with microbiologists, plant physiologists and the commercial greenhouse grower community from UC Santa Cruz, NASA Ames, and Monterrey Bay Farms. Corrado developed materials for luminescence solar concentrators (LSCs) and studied photovoltaic (PV) technologies and the spectral dependence of plants to enable PV to coexist with agriculture land use for both food and biofuel production (see Fig. 2). She was instrumental in developing greenhouse integrated photovoltaics (GIPV) through NSF's Innovation Corps (I-Corps™) program that fosters entrepreneurship and technology commercialization.<sup>14</sup> With the launch of a start-up company, Soliculture, they produce "power-generating greenhouse panels that absorb wavelengths of light in the green region of the spectrum, where plants do not absorb efficiently, and

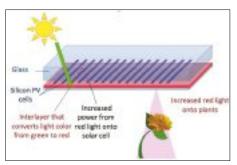


Fig 2. Cartoon illustrating the concept behind the panels that Dr. Corrado helped to produce for use in greenhouse integrated photovoltaic (GIPV) technology.

emit light in the red region of the spectrum to simultaneously enhance light quality onto plants as well as power production by solar cells." This example illustrates how material scientists are thinking broadly about their fundamental research at a "systems-level".

# Resilience and Adaptability

Resilience and the ability to adapt to changes are also important to society. Prediction of natural or anthropogenic disasters and similar events such as hazardous earthquakes and severe storms engage sensors, sensor networks, and employ computations and models. Known elements, for instance the environmental degradation of the structural integrity of bridges and other civil infrastructures, call for materials innovation, e.g., in sensors and self-healing materials. Seasonal and long term road deterioration also demands more adaptable materials.

Sustained human health and well-being is paramount to the quality of life. Much effort goes into prediction or early detection of disease or problems and their prevention, and to the treatment of injuries. The White House's BRAIN<sup>15</sup> and Neuroscience<sup>16</sup> Initiatives are just a few of the newest steps in this direction that include a clear focus on obtaining a better understanding of the body. It remains a sought after goal to better understand regeneration and autophagy (natural degradation processes within the human body). Moreover, it is desirable that treatments be targeted at the ailment and avoid deleterious effects systemically on the body or other non-affected regions.

Additive manufacturing has provided resurgence in creating replacement parts. Similarly, research on the development of new technologies for persons with disabilities continues to be important. Research directed toward the characterization, restoration, and substitution of functional abilities/cognition includes both neuroengineering and rehabilitation robotics.



Fig 3. Molecular model of a newly discovered hybrid polymer showing the two supramolecular domains that can be assembled and disassembled, with significant potential for future technologies using self-healing materials.

One recent NSF-funded breakthrough that could have applications for both self-healing and drug delivery materials was reported by Professor Samuel Stupp at Northwestern University (Fig. 3). He pioneered the synthesis of polymers simultaneously using both chemical synthesis and self-assembly.<sup>17</sup> His approach has resulted in new materials with nanoscale sized

compartments that can be disassembled and reassembled at will, which brings us closer to mimicking Mother Nature and could be a breakthrough for applications in self-healing materials. Material researchers need to facilitate the transition of such important fundamental discoveries into advanced technologies that have societal benefits.

# Advanced Manufacturing

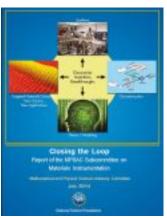


Fig 4. The report cover for "Closing the Loop - Report of the MPSAC Subcommittee on Materials Instrumentation," a concept inspired by the Materials Genome Initiative and being implemented in projects supported by DMREF and MIP programs.

Modern sophisticated, efficient, clean and state-of-the-art manufacturing has recently garnered widespread interest. For example, in 2011, President Obama announced three new national initiatives, Materials Genome Initiative (MGI), Advanced Robotics Initiative and the Advanced Manufacturing Initiative.18

NSF responded to MGI through creation of Designing Materials to Revolutionize and Engineer our Future (DMREF) program.<sup>19</sup> The premise for this program is the fact that advances in computation/modeling/simulation characterization tools are now at a point that we are generating so much data, it is prudent to

rethink the way we conduct research. DMREF is leading this culture shift in materials research by encouraging and facilitating an integrated team approach through what we describe as, "cyclic synergism" or "closing the loop"(Fig. 4)<sup>20</sup>. This "MGI approach", as stated in the federal interagency MGI Strategic Plan<sup>21</sup>, seeks to uniquely and seamlessly integrate computation, experiment and data to fuel the successful discovery of new materials and their more rapid deployment and incorporation into manufactured products" (see Fig. 5). DMREF challenges the materials research community to integrate, experiment, computation and theory iteratively (cyclic synergism) rather than in parallel (linear synergism) to enhance information flow and advance our ability to design and make materials with specific and desired functions or properties from first principles. The DMREF teams are also challenged to integrate digital data, software and program outputs into the wider materials community.

For example, a DMREF project led by Professor Chang-Beom Eom at the University of Wisconsin successfully applied this cyclic synergism approach and discovered general design rules for "polar metals".22 Previously it was believed that a combination of these properties (i.e., metallic and polar) was not possible; however through a new synthesis approach supported by computational modeling, the group made a crystal that was part polar, part metallic, opening up possibilities for advanced materials with the ability to perform simultaneous electrical, magnetic and optical functions.

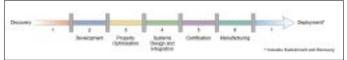


Fig 5. Materials Development Continuum as described by the Materials Genome Initiative Strategic Plan.

The "MGI approach" was key to this discovery process, but the materials research community will need to expand this approach further to the systems-level. Material researchers must transcend the parallel materials development continuum displayed in Fig. 5 and iterate, not just at the discovery stage, but also apply cyclic synergism between all stages of the materials development continuum; only then can the promise of MGI and its benefits to society be realized.

# **Quality of Life**

Moreover, quality of life is affected by how our time is used. As alluded to already, time should not simply be eroded away by maintenance and repairs, nor should it be wasted, i.e. spent commuting, making repetitive movements in manufacturing, and through inefficiencies associated with obtaining leisure time and recreational activities. We are just beginning to see how self-driving cars will alter commuting, but it is uncertain how road congestion and wear, and emergency care will be affected. Robotics can remove dangerous and repetitive steps in manufacturing; however, the public is still adapting to a modern vision of manufacturing operations today. Technology advances permit virtual visits to museums and natural wonders, and remote conversations are now easily visual as well as auditory. However, virtual group meetings can still be cumbersome (as an amusing YouTube video<sup>23</sup> illustrates). Technological developments are needed to improve these advancements and cognitive sciences are key to their full integration and acceptance in society.

# HISTORY OF MATERIALS RESEARCH AND THE NATIONAL SCIENCE FOUNDATION (NSF)

Academic departments at U.S. universities and colleges dedicated to the study of materials science and engineering began in the 1950's. An early adopter was Northwestern University whose faculty members in the metals department recognized that the study of materials using the "processing-structure-properties" paradigm could be and should be applied to other materials.<sup>24</sup> In the 1960's and 1970's, the Advanced Research Projects Agency (ARPA), later known as the Defense Advanced Research Project Agency (DARPA), created Interdisciplinary Research Laboratories (IRLs) as part of their mission "to make pivotal investments in breakthrough technologies for national security.<sup>25</sup> While the IRL concept contributed further to the growth and acceptance to the study of materials as a field of research, it was realized that in order for this "mode of operation", to be successful, longer-term investment was necessary. The IRLs, originally created to support interdisciplinary research in materials science for national security, were transferred to NSF in 1972 to align with a broader set of national needs and to secure longer-term funding. This shift was described as the "first serious effort to induce group activity in academic research....when NSF assumed responsibility for the materials laboratories formerly known as IRLs"26 and created the Division of Materials Research (DMR). These materials laboratories still exist today as the divisional flagship program, the Material Research Science and Engineering Centers (MRSECs), with the mission:

"to undertake materials research of a scope and complexity that would not be feasible under traditional funding of individual research projects. NSF support is intended to reinforce the base of individual investigator and small group research by providing the flexibility to address topics requiring an approach of broad scope and duration."<sup>27</sup>

In addition to the MRSEC program and national facilities (National High Magnetic Field Laboratory (NHMFL) and the Cornell High Energy Synchrotron Source (CHESS)) that underpin a broad set of experiments for science and engineering research, DMR currently houses five "material type" programs (Biomaterials, Ceramics, Electronic and Photonic Materials, Metals and Metallic Nanostructures, and Polymers) and three broad "disciplinary" programs (Condensed Matter Physics, Condensed Matter and Materials Theory, and Solid State and Materials Chemistry). These topical programs allow individual investigators (primarily from academic institutions in the U.S.) to submit unsolicited research proposals for consideration and to have access to a diverse set of characterization tools.

While materials research originated with studies of traditional materials such as ceramics and metals, over the last 50 years it has significantly expanded to include polymers, biomaterials, nanomaterials (although not "new", better understood in modern times), quantum materials, mesomaterials, metamaterials, etc. – a vast mixture, or motley, of solid substances. Over the last two decades, programmatic composition of DMR has evolved to be more inclusive of the changing materials landscape (e.g., Biomaterials was added as a program, and other programs underwent expansions reflected in their name changes: Solid State Chemistry added "Materials Chemistry", Condensed Matter Theory added "Materials Theory" and Metals added "Metallic Nanostructures").

More recently, advances in materials modeling, theory and data mining and the potential for acceleration of materials discovery and deployment, as envisioned by MGI laid the basis for two new DMR programs, DMREF and Materials Innovation Platforms (MIPs).<sup>28</sup> The DMREF program, described earlier, is led by DMR and includes numerous divisions at NSF in three directorates (Mathematical & Physical Sciences, Engineering, and Computer & Information Science & Engineering). The MIP program was launched in 2015, and takes the MGI-approach (i.e., cyclic synergism) to a larger scale by combining a focused research effort with a mid-scale user facility to advance materials topics of national need. These platforms respond to the increasing complexity of conducting materials research that requires close collaboration of multidisciplinary teams who have access to cutting-edge tools and experts in material synthesis, characterization and theory, and makes available shared samples (e.g., single crystals, films, software, data sets). The success of the MIPs, to accelerate our ability "to discover, manufacture, and deploy materials in half the time at half the cost" as envisioned by MGI, will strongly depend on the development of a "community of practitioners" (i.e., enabling the research community to use these central facilities, as well as apply the MGI mode of operation to advance the platform's goal). Two such platforms were awarded in 2016, to Penn State University (Two-Dimensional Crystal Consortium (2DCC)) and Cornell University (Platform for Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)). MIPs will serve as focal points that promote cross-fertilization of ideas between researchers (both internal and external) thanks to their unique convergence of facilities and expertise.

# **DIVERSITY OF IDEAS AND PEOPLE**

When biologists think about diversity they consider the variety of species, ecosystems and ecological processes on a global basis. Material researchers also talk about diversity. In doing so, they are reaching for and seeking a diversity of ideas. One aspect of diversity







Fig 6. Participants in the PREM award between University of Puerto Rico-Humacao and the University of Pennsylvania MRSEC are shown participating in research and learning activities. The Principal Investigators of this award promote early research experiences, mentoring, networking and role models to promote women in Physics and Computational Mathematics.

is in terms of approach: theory, computation, data, experimentation, and manufacturing production. Diversity of perspective is also important - the keys to how things work (that fundamental understanding), how details fit into a larger system, and the efficiency of processes. Material researchers are also considering sustainability, adaptability to different scenarios, cost reduction, manufacturability, technology transfer and added value to society. Finally, material researchers are seeking diversity in backgrounds - formal education, ways of thinking, and the ability to relate to more than one (science) language (a key aspect to nanotechnology that bridged many traditional disciplines). But, also, equally important for these complex problems we face today, is a diversity of life experiences. These bring a different understanding to societal problems and ideas for solutions. Well known are the positive effects of bringing women into design teams that yield a product more relevant to the entire breadth of consumers. This sentiment applies equally well to all underrepresented groups.

While DMR encompasses the mix of disciplines necessary to address materials research challenges, it also promotes diversity of people. All MRSECs and facilities have a diversity plan as part of their function. In addition, the Partnership in Research and Education in Materials (PREM) program was launched in 2004 with the objective to broaden participation and enhance diversity in materials research and education by stimulating the development of formal, long-term, multi-investigator, collaborative research and education partnerships between minority-serving colleges and universities and MRSECs and facilities (Fig. 6).<sup>29</sup> The PREM program is first and foremost a competitive research award that also emphasizes important elements such as mentoring, capacity-building and shrewd networking.

Just imagine for a minute that you are tasked with solving a problem where you do not clearly understand the issues, or you do not have all of the skills needed...can you do it effectively on your own? Of course not! The expression, it takes a village, is popular for a reason.

# References

- 1 http://www.greatachievements.org/
- 2 http://www.greatachievements.org/?id=3805
- Grand Challenges for Engineering, National Academies, 2008, Washington D.C.
- 4 https://www.whitehouse.gov/the-press-office/2015/12/12/us-leadership-and-historicagreement-combat-climatechangehttps://www.whitehouse.gov/sites/whitehouse. gov/files/documents/
- https://www.whitehouse.gov/sites/whitehouse.gov/files/documents/White\_House\_ Water\_Summit\_commitments\_report\_032216.pdf
- https://www.whitehouse.gov/blog/2012/04/12/sustainable-farming-global-and-nationalfood-security5
- https://www.whitehouse.gov/blog/2010/09/27/educating-next-generationenvironmental-stewards
- Materials for Sustainable Development, MRS Bulletin, vol. 37, No. 4, April 2012.
- L.D. Madsen and A.A. White, "Investments in Ceramic Science, Engineering and Education for Sustainability by the US National Science Foundation", J. Electroceram. 32: 60-65, DOI: 10.1007/s10832-013-9851-7 (Jan. 2014).
- 10 http://www.nsf.gov/funding/pgm\_summ.jsp?pims\_id=504707
- A.A. White, M.S. Platz, D.M. Aruguete, S.L. Jones, L.D. Madsen and R.D. Wesson, "The National Science Foundation's Investment in Sustainable Chemistry, Engineering, and Materials", American Chemical Society Sustainable Chemistry & Engineering, 1 (8), 871–877, http:// dx.doi.org/10.1021/sc400002r (2013).
- 12 http://www.nsf.gov/publications/pub\_summ.jsp?ods\_key=nsf15085
- 13 https://www.nsf.gov/funding/pgm\_summ.jsp?pims\_id=504673
- 14 http://www.nsf.gov/news/special\_reports/i-corps/
- 15 https://www.whitehouse.gov/share/brain-initiative
- 16 https://www.whitehouse.gov/administration/eop/ostp/initiatives
- 17 Z. Yu, F. Tantakitti, T. Yu, L.C. Palmer, G.C Schatz, and S.I. Stupp, "Simultaneous covalent and noncovalent hybrid polymerizations", Science, 351(6272) 2016
- 18 https://www.whitehouse.gov/the-press-office/2011/06/24/president-obama-launchesadvanced-manufacturing-partnership
- 19 http://www.nsf.gov/funding/pgm\_summ.jsp?pims\_id=505073
- 20 http://www.nsf.gov/mps/advisory/mpsac\_other\_reports/subcommittee\_report\_mi\_final.pdf
- https://www.whitehouse.gov/sites/default/files/microsites/ostp/NSTC/mgi\_strategic\_ plan\_-\_dec\_2014.pdf
- T.H. Kim, D. Puggioni, Y. Yuan, L. Xie, H. Zhou, N. Campbell, P.J. Ryan, Y.Choi, J.-W. Kim, J.R. Patzner, S. Ryu, J.P. Podkaminer, J. Irwin, Y. Ma, C.J. Fennie, M.S. Rzchowski, X.Q. Pan, V. Gopalan, J.M. Rondinelli, and C.B. Eom, "Polar metals by geometric design", doi:10.1038/ nature17628

- 23 https://www.youtube.com/watch?v=DYu\_bGbZiiQ
- 24 http://www.mccormick.northwestern.edu/magazine/fall2005/MSE.html
- 25 http://www.darpa.mil/about-us/darpa-history-and-timeline
- 26 http://www.nsf.gov/attachments/118193/public/LookingBackMovingForwardNSF sMRSEC.pdf
- 27 http://www.nsf.gov/funding/pgm\_summ.jsp?pims\_id=5295
- 28 http://nsf.gov/pubs/2015/nsf15522/nsf15522.htm
- 29 http://www.nsf.gov/pubs/2014/nsf14606/nsf14606.htm



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