# Interdisciplinary collaboration, robust funding cited as key to success of Materials Genome Initiative program

www.whitehouse.gov/mgi

The US government's Materials Genome Initiative (MGI), now in its third year, seeks to significantly reduce the time and cost of bringing new materials from the laboratory to the marketplace through enhanced integration of computation, experiment, and digital data. The National Science Foundation (NSF), one of the main agencies participating in MGI, supports the initiative through its Designing Materials to Revolutionize and Engineer our Future (DMREF) activity. The program funds collaborative and iterative approaches to materials design in which computation guides experiment and theory, which in turn further advance computation. NSF invested over USD$12 million in the program's first round of awards to support 14 projects in Fiscal Year (FY) 2012, and recently announced over USD$22 million in awards for FY 2013 to support 19 projects.

The DMREF awards made thus far cover a wide range of basic materials science and engineering topics, from fracture behavior in metallic alloys and functional materials for spintronics, to anisotropy in organic glasses and self-assembling peptide nanotubes. The projects are typically collaborations between several principal investigators (PIs) that are three to four years in duration.

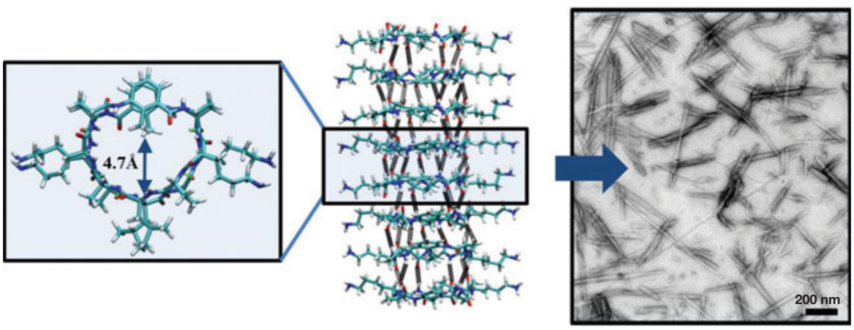
For most researchers who received a first-round award, the intimate, interdisciplinary, and often large collaborations DMREF engenders have been the keys to scientific success. Haitham El Kadiri, a professor at Mississippi State University, is part of a four-PI team working to develop and verify models capable of predicting failure in Mg alloys. "The problem we're addressing is so complex you need a large group with a range of expertise," said El Kadiri. "It would be almost impossible for a single research group to tackle this."

For Ting Xu of the University of California–Berkeley, and Sinan Keten of Northwestern University, the combination of experiment and theory has enabled them to be successful and efficient in understanding the way different conformations of peptides stack to form nanotubes for use in selective membranes. "Seeing Sinan's visualization of how our systems are working provides more certainty about which direction to take my experiments," said Xu. Keten then uses Xu's experimental work to verify each new round of models. "Seeing the benefits of this approach, I've changed the way I'm carrying out my research," Keten said. "I now want to incorporate experimental aspects into each of my projects."

While the projects have made progress integrating theory and experiment, for most the iterative component will have to come later. "Large collaborations like this have a bit of a start-up time," said Darrin Pochan of the University of Delaware. "You have to hire all the necessary personnel and buy equipment, and you have to spend time talking about your individual capabilities and your joint goals for the project." Pochan, one of three PIs on a DMREF project looking at peptide self-assembly, also said that computational components often need lead times, too, particularly in the case of soft materials. "With inorganic electronic materials, theory historically has been a much more intimate part of new materials development. Partly due to the complexity of biomaterials systems, there has been no direct theory component, so fundamental solution theory and corresponding simulation code have to be developed first."

Those who have experienced the MGI approach in their research see clear benefits. "I'm hopeful based on our first-year experiences that this can, in fact, revolutionize things," said Pochan. "There will always be experimental serendipity, but theoretical guidance will make it quicker." David Vanderbilt, a Rutgers University professor who received funding from DMREF, appreciates the approach and goals of MGI, but is more cautious about the transformative power of the program itself. "It's useful to have MGI as an ambitious goal, and it can have a significant impact if the ideas propagate throughout the community more generally, but the program's funding isn't of sufficient scale to drive a transformation by brute force."

Indeed, large-scale programs are difficult to advance with sequestration currently in effect. Recognizing the tough budgetary decisions NSF will likely continue to face, many stress the importance of maintaining grant award values at a suf-




Characterization of cyclic peptide nanotubes through joint efforts combining simulations with experiments. Courtesy S. Keten and T. Xu.

ficient level to carry out the work. "To do this kind of research correctly, you need a full effort on all the pieces," said Pochan. "There are three labs involved in our project, so you need three times the funding."

Some DMREF-funded researchers, particularly those looking at very fundamental science, emphasize the unique opportunity these large collaborative grants provide. "There would be nothing else to fund this project if not for DMREF," said El Kadiri. Keten agreed, and said MGI should be a top funding priority, but he also highlighted that single-PI grants "can provide crucial advances in areas where overlap between experiment and theory is virtually non-existent."

DMREF has yet to become a top funding priority. NSF's FY 2014 budget request slated a modest USD$42 million for DMREF across the Foundation, with the Directorates for Engineering; Mathematical and Physical Sciences; and Computer and Information Science and Engineering expected to participate. Furthermore, in the current fiscal climate, the program's enacted budget may be considerably less, and thus a materials evolution may be more likely than a revolution.

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## National Academies recommend single-agency oversight of nanomaterials safety

http://national-academies.org

While some progress has been made in advancing the US research agenda on environmental, health, and safety aspects of engineered nanomaterials, little work has been done in implementing an integrated research strategy throughout the federal government, according to a report from the US National Research Council. The report, *Research Progress on Environmental, Health, and Safety Aspects of Engineered Nanomaterials*, suggests that progress could be accelerated if a single agency with sufficient management and budgetary authority was designated to direct environmental, health, and safety research efforts and ensure implementation of a coordinated plan among the federal agencies that make up the National Nanotechnology Initiative (NNI).

The global market for nanotechnology is expected to exceed USD$3 trillion by 2015, including products ranging from cosmetics to medical therapies to electronics. The unique characteristics and behaviors of nanomaterials and uncertainties regarding how they interact with biologic systems have spurred research on their potential risks to human health and the environment. However, despite an increase in funding and peer-reviewed publication of research over the past decade, environmental, health, and safety