Third NSF decadal report presents challenges for polymer field

By **Arthur L. Robinson**

"For the polymer community, this is huge. It is the third such study, each charting the key challenges for the field in the coming decade," says Richard Vaia of the Air Force Research Laboratory at Wright-Patterson AFB, Ohio, on the recently released report of an August 2016 National Science Foundation (NSF) workshop "Frontiers in Polymer Science and Engineering." Vaia joined workshop initiator Andrew Lovinger of NSF and Kathryn Beers of the National Institute of Standards and Technology in supporting workshop chair Frank Bates of the University of Minnesota, Twin Cities, and a cadre of workshop co-organizers. More than 70 workshop participants spanned the range from academic to industrial and government researchers.

The report is notable because it spans the entire field of polymer science and engineering. "The polymer scope is enormous, and it's only getting bigger," says Bates, "so it was once again timely to evaluate the field in its entirety, including a look at how it impacts science and society." For all three decadal polymer overviews, Lovinger sought the co-sponsorship of several federal agencies supporting polymer research. "I wanted these workshop reports and their recommendations to be seen not just as reflecting NSF priorities, but as indicative of the interests of agencies across the government," he says.

The two prior workshop reports were very prophetic. Many of the challenges and opportunities identified evolved into major efforts within the polymer community and also across a wider range of research fields. Starting with the monomers from which they are constructed, polymers fit naturally into the nanoworld, and the 1997 report had nanoscience as one theme. Its recommendations anticipated initiatives at NSF and elsewhere as the nano-revolution was taking hold throughout the research world. Similarly, the 2007 report highlighted the importance of energy and environmental sustainability, cornerstones of subsequent NSF initiatives in solar energy and sustainable chemistry and materials. And they continue to draw widespread attention today.

Where will the 2017 report have the biggest impact? NSF's Lovinger is making no predictions. "We are trying to grow the entire field without giving the impression that we have favorites," he says. For those seeking clues to the future, the report's Executive Summary identifies four broad themes and overarching concepts that resonated with the workshop's participants: Integration from nanometers to meters, advanced instrumentation, ubiquitous theory and computation, and bridging the academia–industry divide. The executive summary in the report also lists scientific and engineering themes that cross through the eight sections in the document. Each section, in turn, identifies "grand challenges" and concludes with its own set of recommendations (see Table I).

Of the four broad themes identified in the Executive Summary, Bates calls attention to the transition of theory (computation and simulation) from a separate subject to one inextricably bound to experiment. "Theory is important in every area of polymer science and engineering," said Bates, "and it needs to be in concert with experiment through the formation of close collaborations." Bates cites the example of precision chemistry (Section 2: Macromolecular Synthesis), where there have been major advances in the synthesis of large molecules, as a probable beneficiary of close collaboration with theorists. "Chemists can make almost anything," he said, "and they are now aiming to rival what can be done in the biological world. Combining this kind of precision chemistry with theory and simulation will create engines for innovation and discovery."

The Air Force's Vaia agrees, noting an exciting convergence among (1) simulation and big data to frame the complexity of polymers that arises from their hierarchy of structure and relaxation times; (2) chemistry, where techniques are developing toward sequence specific control; (3) biochemistry, where synthetic and systems biology are enabling microbes to synthesize fine chemicals; and (4) characterization tools that enable detailed (location specific) nanoscale insights into composition, structure, and processes. "Together these are the four critical components of a revolution in molecular-level engineering."

Section 3 (Hierarchical Structures at Multiple Length Scales and Energy Scales), for example, points out that polymers are capable of simultaneously achieving order over a wide range of length scales. These hierarchical assemblies form due to an interplay between thermodynamic and kinetic driving forces acting through the atomic (monomer), nanoscopic (monomer sequence, chain shape), and mesoscopic length scales. Order at every length scale affects both the structure and function of the resulting polymers. "Those forces acting on the microscopic functional groups have to be transferred and amplified via hierarchical structures at different length scales to generate the macroscopic properties," says Stephen Cheng of The University of Akron. "Therefore, designing building blocks and assembling modules via different interactions are the key pathways to creating new polymer materials."

While the future looks promising for the field, many challenges remain. Murugappan Muthukumar of the University of Massachusetts Amherst, names the nonequilibrium (and hierarchical) structure and dynamics of polymers as one of the major ones. "There is a lack of understanding [of nonequilibrium effects] in the polymer field," he says, giving polymer crystallization as an example. "There is a hierarchy over energy, length, and time scales of nonequilibrium assemblies emerging from baby nuclei that grow and decay, with survivors becoming

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intertwined and entangled in the course of folding many times before reaching a semicrystalline state." Semicrystalline means that there are coexisting regions of crystalline order and amorphous disorder. Even for polyethylene, one of the simplest and most widely produced polymers, there still is no proper theory of crystallization.

The fourth of the broad themes and challenges, bridging the academia–industry divide, resonated with Shenda Baker of Synedgen, a startup in Claremont, Calif. Today's leaner corporations are focused on quarterly bottom lines and, for the most part, have de-emphasized long-term research and close collaboration with academic researchers. Moreover, the rise of entrepreneurialism has generated a host of companies that are fonts of innovation, if they survive, but are too small to support research facilities that cutting-edge research requires. Finally, the most expensive facilities, such as synchrotron and neutron-scattering sources, are most often found in government-funded national laboratories. "How can we bridge the broadening gap between the industrial and the academic and government worlds?" Baker asked. Recommendations in Section 6 (Partnerships: Academia, Industry, and Government) of the report cover a wide range of topics, from creating templates for reasonable intellectual property agreements to establishing government-funded characterization, manufacturing, and polymer research centers in universities.

Table I. Grand challenges for each of the eight sections of the report "Frontiers in Polymer Science and Engineering."

1. **Societal Impact** • Environmental Impacts • Energy Applications • Infrastructure, Communications, and Information • Food/Water/Air • Health • Aspirational and Curiosity-Driven Needs	Six areas of overarching opportunities and challenges: • Achieve accessible, scalable polymers that match or exceed the property matrix of existing materials, yet have a green life cycle. • Energy storage and generation materials with a combined 10x improvement in cost, properties, and performance. • Rapid, low-cost, local production of lightweight, robust infrastructure. • Combined 100x improvement (cost, efficiency) in new purification materials and the development of biodegradable, smart, high-barrier polymers for food packaging. • Innovative materials development for cost-effective infectious disease control, treatment, and diagnostics. • Invest in an environment that allows and encourages scientists, engineers, and entrepreneurs to pursue bold, transformative ideas and think outside the box.
2. **Macromolecular Synthesis**	Macromolecular syntheses that afford the opportunity to create an infinite spectrum of tailored molecular architectures.
3. **Hierarchical Structures at Multiple Length Scales and Energy Scales**	To make the next leap in designing functional materials, we must understand, predict, and use molecular building blocks, sequence, conformation, and chirality to direct mesoscopic structure at desired time and energy scales to control macroscopic polymer properties.
4. **Integrated Measurement, Analysis, and Prediction**	To develop new tools—experimental and computational methods and theory—and leverage them in an integrated way across any relevant length scales and time scales to accurately measure, predict, and elucidate underlying connections among structure, properties, and dynamics of any macromolecular system.
5. **Advancing Performance**	Advancing polymer performance requires simultaneous control over multiple orthogonal properties through rational material design, often in combination with other system components; and through robust, controllable processing methods.
6. **Partnerships: Academia, Industry, and Government**	Establish practical and efficient mechanisms that foster cooperation, collaboration, and working partnerships between industry, academia, and government agencies and national laboratories for the purpose of advancing basic research and technology development.
7. **Higher Education and Diversity**	Design an education that embraces the breadth and complexity of polymer science and engineering and delivers it to a diverse student body, making full use of technology to exploit expertise across the field.
8. **Outreach and Broadening Participation**	To "raise" a diverse community of future scientists and interested citizens. This requires efforts that begin with young children and their families, and continues through to launching ambitious high school graduates toward university and beyond.

Diversity is one issue that polymer science and engineering shares with other scientific communities. In particular, the report points out, "The makeup of the scientific community does not match that of the US population nor even the profile of college students nationwide." The problem is both one of implicit and explicit bias in hiring and retention (Section 7 – Higher Education and Diversity), as well as failure of the educational system to attract a large segment of the student population to science at an early age (Section 8 – Outreach and Broadening Participation). A comment concerning implicit bias cuts to the chase: "This is not a conversation that happens easily, but it needs to happen, or the strategies [we have discussed] will not lead to real change."

Although not a grand challenge itself, improving public perception of polymers has proven to be a vexing problem. "Everybody knows about plastics and rubber," says Bates, "but they don't know about the impact that polymers are having in every sphere of science and engineering, not to mention life itself." The report admirably summarizes the pervasiveness, importance, and economic impact of polymers, now a nearly USD$500 billion global market, in Section 1 (Societal Impact): There is hardly any aspect of our life today that is not affected and improved by polymers, and it would be fair to characterize this era as the "polymer age."

Copies of the report are available from stone094@umn.edu, or electronic versions can be downloaded at https://z.umn.edu/nsfpolymerworkshop2016.

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