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Research domain(s), discipline(s)/sub-discipline(s)

Professional societies; Ceramic and glass materials science and engineering

Title of Response

A collaborative approach to building a cyberinfrastructure and workforce for materials science

Abstract

The materials science discipline spans a wide range of materials with a commensurately wide range of data types, ranging from property data, to crystal structures, to microstructures and more. Building a cyberinfrastructure for the materials science community requires bringing together the primary disciplines of ceramics, glasses, metals, and engineering polymers, and their various subdisciplines. The

effort requires long-term leadership and vision to unify the collective materials science community. Professional societies are uniquely able to serve this role.

Question 1 (maximum 400 words) – Data-Intensive Research Question(s) and Challenge(s). Describe current or emerging data-intensive/data-driven S&E research challenge(s), providing context in terms of recent research activities and standing questions in the field. NSF is particularly interested in cross-disciplinary challenges that will drive requirements for cross-disciplinary and disciplinary-agnostic data-related CI.

Demand for new materials with extraordinary functionality creates an urgent need for use of rapid discovery and refinement techniques. Data-driven methods, encompassing tools such as machine learning, artificial intelligence, and big data informatics, offer a new paradigm for researchers to discover new glasses and ceramics efficiently and effectively. Development of close collaborations between data science and materials science research communities is an essential element of realizing the objective. Leaders in the glass and ceramic research community already are embracing data science and informatics tools to study complex materials, processes, and applications. Key collaborative challenges to solve include bridging physics-based, empirical, and data-driven models; creating collaborative data infrastructure; boosting interdisciplinary education; and enhancing data usability and visualization. Solutions to these challenges will require fluency in data science as well as materials science. Glass and ceramic researchers will need near-expert proficiency in data science and informatics, and vice-versa, making education in data science methods increasingly important for glass and ceramic researchers. Universities and professional societies are best-positioned to respond to this need with input from industrial customers.

Question 2 (maximum 600 words) – Data-Oriented CI Needed to Address the Research Question(s) and Challenge(s). Considering the end-to-end scientific data-to-discovery (workflow) challenges, describe any limitations or absence of existing data-related CI capabilities and services, and/or specific technical and capacity advancements needed in data-related and other CI (e.g., advanced computing, data services, software infrastructure, applications, networking, cybersecurity) that must be addressed to accomplish the research question(s) and challenge(s) identified in Question 1. If possible, please also consider the required end-to-end structural, functional and performance characteristics for such CI services and capabilities. For instance, how can they respond to high levels of data heterogeneity, data integration and interoperability? To what degree can/should they be cross-disciplinary and domain-agnostic? What is required to promote ease of data discovery, publishing and access and delivery?

In 2015-2017, The American Ceramic Society (ACerS) led a NIST Advanced Manufacturing Technology project to plan for the launch of the Functional Glass Manufacturing Innovation Consortium (FGMIC) and develop the roadmap, Driving Functional Glass Manufacturing Innovation: A Technology Roadmap to 2025 (https://ceramics.org/professional-resources/functional-glass-manufacturing-innovation-consortium). The roadmapping process identified the need for increased coordination between the glass community and the data science and informatics community, and this need cut across all aspects and priorities of the roadmap. Key benefits to the application of data science to glass include: • Tailored properties: By generating structure-property data from characterizations coupled with modeling and existing glass databases, manufacturers will gain an increased understanding of the structural characteristics of glasses, enabling them to more accurately develop glasses with improved functionality, more consistent and reliable performance, and reduced costs. • Development of new glass compositions: Using well-established glass theory and simulation, coupled with data-driven glass informatics for information sifting or screening (the driving concept of the Materials Genome Initiative), can help narrow down the essentially infinite glass composition space. • Improved process control: The sophisticated combination of heterogeneous data from varied theoretical calculations, empirical modeling, and processing characterizations will help companies pinpoint opportunities for maximizing process efficiency, which can reduce product development time and minimize manufacturing costs. While this funded project focused on glasses, ample evidence in ACerS journal articles, conference symposia, and a Society technical interest group pointed to a similar need for data science and informatics in the ceramic science research community. ACerS convened a workshop in Feb. 2018 to address the need for collaboration between the data science and glass/ceramic communities. The one-day workshop brought together a select group of more than 20 experts in the data science, informatics, and ceramic/glass communities from industry, universities, national laboratories, government agencies, and ACerS to discuss and prioritize opportunities and mechanisms for increasing collaboration and coordination between these communities. Care was taken to evenly balance expertise in data science/informatics and ceramic/glass science to avoid “silos,” encourage diversity of thought, and uncover challenges and opportunities that tend to be invisible within discrete communities. The 2019 paper, “Data-driven glass/ceramic research: Insights from the glass and ceramic and data science/informatics communities,” in the Journal of the American Ceramic Society (DOI: 10.1111/jace.16677) reports the challenges and opportunities identified and prioritized by workshop participants. The workshop findings comprise representative views of the data science/informatics communities and ceramic/glass communities. The workshop pointed to the need for interdisciplinary education that integrates data science into materials science education, and vice versa. On the subject of infrastructure, participants identified the need for collaborative solutions. The data science/informatics community’s top five challenges with respect to materials science were 1. Lack of infrastructure and data sharing, 2. Lack of appropriate computational approaches to glass and ceramic materials questions, 3. Insufficient cultural and educational support, 4. Limited data accessibility and usability, 5. Lack of data reliability and quality control. The ceramic/glass research community’s top five challenges with respect to embracing data science/informatics were 1. Difficulty bridging physics-based, empirical, and data-driven models, 2. Need for workforce training and education, 3. Inadequate data fusion approaches, 4. Lack of data infrastructure, 5. Limited industry communications and interaction. Out of this discussion, the participants identified and prioritized four opportunities for collaboration between the glass and ceramic and data science and informatics communities: 1. Bridging physics-based, empirical, and data-driven models, 2. Creating collaborative data infrastructure, 3. Boosting interdisciplinary education, 4. Enhancing data usability and visualization.

Question 3 (maximum 300 words) – Other considerations. Please discuss any other relevant aspects, such as organization, processes, learning and workforce development, access and sustainability, that need to be addressed; or any other issues more generally that NSF should consider.

We strongly encourage the NSF to consider the benefits of enlisting professional societies to bring together disparate disciplines and organizations. The idea of establishing collaborations or consortia typically emerges at data workshops. We suggest the most effective collaboration or consortium would be between professional societies representing the memberships of the disciplines that should be engaged to build a cyberinfrastructure and develop a data-fluent materials science workforce. Professional societies were founded to advance their industry's needs, and their membership networks extend across all organization types: academia, government, industry, and nonprofits. By design, professional societies serve as neutral advocates and offer an environment wherein entities with competing interests can work together for the mutual benefit of the discipline or industry. Societies operate with a long-term view and have developed committees and other organization structures to ensure long-term continuity in their activities. Also, professional societies have a long history of collaboration. For example, alloy designations and specifications were developed by industry through associations and professional societies. Finding all existing materials data repositories is in itself a herculean task. Many subdisciplines of materials science steward and use specialized databases of high value to their community, but unknown outside of the community. Professional societies, through their members, have the ability to discover these databases and bring them into the collection of data resources. Finally, professional societies have the organizational competencies to organize and run working groups, workshops, conference symposia, and they have the channels at their disposal to inform the communities involved through online and print media.

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