The Department of Chemical Engineering Presents:

Polymer Informatics: Current Status & Critical Next Steps

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https://rochester.zoom.us/j/98875611576?pwd=RHY3bmhrRFZEMGhiUW5wZ0VIaDNuUT09

Abstract: The Materials Genome Initiative (MGI) has heralded a sea change in the philosophy of materials design. In an increasing number of applications, the successful deployment of novel materials has benefited from the use of computational, experimental and informatics methodologies. Here, we describe the role played by computational and experimental data generation and capture, polymer fingerprinting, machine-learning based property prediction models, and algorithms for designing polymers meeting target property requirements. These efforts have culminated in the creation of an online Polymer Informatics platform (https://www.polymergenome.org) to guide ongoing and future polymer discovery and design [1-3]. Challenges that remain will be examined, and systematic steps that may be taken to extend the applicability of such informatics efforts to a wide range of technological domains will be discussed. These include strategies to deal with the data bottleneck, new methods to represent polymer morphology and processing conditions, and the applicability of emerging AI algorithms for materials design.

[1] Rohit Batra, Le Song and Rampi Ramprasad, “Emerging materials intelligence ecosystems propelled by machine learning”, *Nature Reviews Materials* (2020) **[2]** Huan Doan Tran, Chiho Kim, Lihua Chen, Anand Chandrasekaran, Rohit Batra, Shruti Venkatram, Deepak Kamal, Jordan P. Lightstone, Rishi Gurnani, Pranav Shetty, Manav Ramprasad, Julia Laws, Madeline Shelton, and Rampi Ramprasad, “Machine-learning predictions of polymer properties with Polymer Genome”, *Journal of Applied Physics* (2020). **[3]** A. Mannodi-Kanakkithodi, A. Chandrasekaran, C. Kim, T. D. Huan, G. Pilania, V. Botu, R. Ramprasad, “Scoping the Polymer Genome: A Roadmap for Rational Polymer Dielectrics Design and Beyond”, Materials Today, 21, 785 (2018).

Bio: Prof. Ramprasad is presently the Michael E. Tennenbaum Family Chair and Georgia Research Alliance Eminent Scholar in the School of Materials Science & Engineering at the Georgia Institute of Technology. His area of expertise is the development and application of computational and machine learning tools to accelerate materials discovery, as applicable to energy production, storage and utilization. Prof. Ramprasad received his B. Tech. in Metallurgical Engineering at the Indian Institute of Technology, Madras, India, an M.S. degree in Materials Science & Engineering at the Washington State University, and a Ph.D. degree also in Materials Science & Engineering at the University of Illinois, Urbana-Champaign. Prof. Ramprasad is a Fellow of the Materials Research Society, a Fellow of the American Physical Society, an elected member of the Connecticut Academy of Science and Engineering, and the recipient of the Alexander von Humboldt Fellowship and the Max Planck Society Fellowship for Distinguished Scientists. He has authored or co-authored over 225 peer-reviewed journal articles, 8 book chapters and 8 patents, and has delivered over 300 invited talks at Universities and Conferences worldwide. He is a member of the Editorial Advisory Boards of ACS Materials Letters and Journal of Physical Chemistry A/B/C, and is the Chair of the inaugural 2022 Gordon Research Conference on Computational Materials Science and Engineering.