USC Viterbi School of Engineering

MORK FAMILY DEPARTMENT OF CHEMICAL ENGINEERING AND MATERIALS SCIENCE

Lyman Handy Colloquia

Presents

Rational Computation-Guided Design of Polymer Dielectrics

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Abstract

To date, trial and error strategies guided by intuition have dominated the identification of materials suitable for a specific application. We are entering a data-rich, modeling-driven era where such Edisonian approaches are gradually being replaced by rational strategies which couple predictions from advanced computational screening with targeted experimental synthesis and validation. Consistent with this emerging paradigm, we propose a strategy of hierarchical modeling with successive down-selection stages to accelerate the identification of polymer dielectrics that have the potential to surpass "standard" materials for a given application. Specifically, quantum mechanics based combinatorial searches of chemical and configurational spaces, supplemented with data-driven (machine learning) methods are used. These efforts have led to the identification of several new organic polymer dielectrics within known generic polymer subclasses (e.g., polyurea, polythiourea, polyimide), and the recognition of the untapped potential inherent in entirely new and unanticipated chemical subspaces offered by organometallic polymers. The challenges that remain and the need for additional methodological developments necessary to further strengthen this rational collaborative design concept are then presented.

Prof. Ramprasad's Bio (http://rampi.ims.uconn.edu/)

After graduating from the University of Illinois at Urbana-Champaign in 1997, Prof. Ramprasad served as a technical staff member at Motorola's R&D division (1998-2004), an Assistant Professor on tenure-track (2004-2009) at the University of Connecticut (his current institution), a tenured Associate Professor (2009-2013), and Professor (2013-current). Prof. Ramprasad's area of expertise is in the development and application of first principles and data-driven materials computational tools, and more broadly in the utilization of such methods for the design and discovery of new materials, especially dielectrics and catalysts. Prof. Ramprasad is a Fellow of the American Physical Society, an elected member of the Connecticut Academy of Science and Engineering. He is the recipient of the UCONN Centennial Term Professorship, the Alexander von Humboldt Fellowship, the Max Planck Society Fellowship for Distinguished Scientists, and the United Technologies Corporation Professorship for Engineering Innovation. Prof. Ramprasad's research is funded by the Office of Naval Research (ONR), the National Science Foundation (NSF), the Department of Energy (DOE), ACS Petroleum Research Fund (ACS-PRF), the Electrical Power Research Institute (EPRI), the Air Force Office of Fundamental Research (AFOSR), and industry. Among other activities, he currently leads a large multi-disciplinary university research initiative (MURI) funded by the ONR aimed at the rational design of capacitor dielectrics using advanced multi-scale computational methods and parallel synthetic routes. He has authored or co-authored over 160 peer-reviewed journal articles, 5 book chapters and 4 patents. He has been a Guest Editor for the Journal of Materials Science, delivered over 150 invited talks at Universities and Conferences worldwide, and has organized several international symposia.

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