WPI MATERIALS SCIENCE & ENGINEERING

Materials Science & Engineering Seminar

Computational Materials Design: Electrocaloric Materials for Waste Heat Recovery

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Washburn 229

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Abstract

There is a need for the development of comprehensive, multi-scale theoretical tools in the search for better materials. This is essentially at the core of the recent "materials genomics/informatics" initiatives that seek to accelerate materials discovery through the use of computations across length and time scales, supported by experimental work. Such methods will result in customizing, or entirely replacing, existing engineering metallic alloys, polymers, and ceramics which were developed based on trial-and-error approaches in the past century. In this talk we will apply these principles to understand pyroelectric, electrocaloric, elastocaloric, and flexocaloric properties of ferroelectric materials. Pyroelectrics can convert heat into electricity by cycling around thermally- and electrically-induced polarization changes, where the energy density scales with the product of the polarization change and applied field. The challenges in realizing caloric energy conversion system are multi-scale and multi-faceted, requiring a combination of first principles computations, phenomenological theory, classical thermodynamics, materials synthesis, and eventually system design [1]. We will discuss our successes and challenges with relating modeled to measured material properties for bulk and epitaxial thin film ferroelectrics. We will provide specific examples related to electrocaloric, elastocaloric, and flexocaloric properties of ferroelectrics [2,3].

Bio:

Dr. Pamir Alpay is the General Electric Endowed Professor in Advanced Manufacturing in the Department of Materials Science and Engineering and Department of Physics of the University of Connecticut (UConn). He is presently the Executive Director of UConn's Tech Park, leading the University's efforts to increase strategic partnerships with businesses in a state-of-the-art research and development facility. Dr. Alpay's research is primarily focused in materials modeling. His research employs a palette of theoretical tools ranging from ab initio computations to basic thermodynamic models. Dr. Alpay is an elected member of the Connecticut Academy of Science and Engineering (CASE) and a Fellow of the American Physical Society (APS) and the American Ceramic Society. He is the recipient of several awards including the NSF CAREER grant in 2001, the UConn School of Engineering Outstanding Junior Faculty Award in 2004, the UConn School of Engineering Outstanding Faculty Advisor Award in 2013 and the AAUP Excellence in Career Research and Creativity Award in 2018. He has over 190 peer-reviewed journal publications and conference proceedings, four invited book chapters, and an invited book co-authored on compositionally graded ferroelectric materials.