THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT WINTER COLLOQUIUM SERIES PRESENTS:

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Patterns in disorder: theory and computation guided prediction of functional properties in complex materials configuration spaces.

Disorder in the atomic configuration of a material refers to a lack of regular patterns or predictability in the atomic positions. The presence of disorder allows us to greatly expand the configuration space available for materials design and functionality. However one consequence of disorder, if the degree is sufficiently large, is the breakdown of conventional descriptions of electronic and vibrational states and transport theories for periodic systems. Hence, computational approaches that are well-established for ordered materials need to be adapted to be able to access functional materials properties in disordered configuration spaces. In this presentation, I will highlight our group's recent work which aims to extend solid-state and semiconductor theory to develop computational approaches applicable to and design rules for disordered materials. The application areas include photovoltaics, thermoelectrics, and materials for chemical energy storage, and we will focus on prediction of properties such as vibrational transport, ion transport, and electronic structure defect chemistry. The principal focus is on development of methods to predict functional properties when disorder is present, validate results with experiment, and use the resulting insights to predict new materials and compositions by design.

Elif Ertekin is an Associate Professor of Mechanical Science and Engineering at the University of Illinois at Urbana-Champaign, and faculty affiliate of the National Center for Supercomputing Applications (NCSA), and the Materials Research Laboratory (MRL) at the University of Illinois. Her research interests are centered on the theory and modeling of materials using a variety of computational methods. She focuses on developing a microscopic understanding of atomic and electronic scale processes, with applications areas in thermal transport, energy conversion, defect chemistry, and disordered materials. She received her PhD in Materials Science and Engineering from UC Berkeley, and carried out post-doctoral work at the Berkeley Nanoscience and Nanoengineering Institute and the Massachusetts Institute of Technology before moving to Illinois. She has received the NSF CAREER Award, the TMS Early Career Faculty Fellow Award, the University of Illinois Rose Award for Teaching Excellence, and recently the 2019 Emerging Leader Award from the Society of Women Engineers.

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