

JEPARTMENT OF MECHANICAI ENGINEERING COLLOQUIUN

UCRIVERSITY OF CALIFORNIA

The Department of Mechanical Engineering PRESENTS

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Disorder Effects on Vibrational Transport in Energy Materials

Abstract:

Disorder in the atomic configuration of a material refers to a lack of regular patterns or predictability in the atomic positions. If the degree of randomness is sufficiently large, one consequence of disorder is localization, which refers to the absence of waves in a disordered medium. The breakdown of the wave picture and the resulting localization of the modes can have strong effects on the electronic, thermal, magnetic, and other properties of materials. In this presentation, I will show some examples from our recent work illustrating the effects of different types of disorder on vibrational transport in energy materials. I will show how established and emerging computational tools can be used to understand the physics that emerges as disorder is introduced. Examples include: the effects of disorder in low-dimensional carbon based materials, hybrid-ordered disordered metamaterials formed by ion beam patterning of silicon, hybrid perovskites which exhibit a dynamic correlated disorder, and diamond-like semiconductors of interest for thermoelectric applications.

About the Speaker:

Elif Ertekin received her PhD in Materials Science and Engineering at UC Berkeley, and then did post-doctoral work at both the Berkeley Nanoscience and Nanotechnology Institute and the Massachusetts Institute of Technology. Her research is centered on the use of computational methods spanning from atomistic first principles to continuum mechanics to describe, predict, and better understand material properties. She has received the TMS Early Career Faculty Fellow Award, the NSF CAREER award, the Dean's Award for Excellence in Research from the College of Engineering at the University of Illinois, and is currently a fellow of the National Center for Supercomputing Applications.