



Dr. Alan McGaughey

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Short Course: Monday, March 14th - 1:00 to 4:00 PM

Virtual Link: <https://cmu.zoom.us/j/6648851369>

Thermal Transport in Messy Systems Interpreted by Molecular Dynamics Simulations

Abstract:

Some ordered materials of scientific and engineering interest are messy, in that they do not have a well-defined unit cell and/or have atoms that do not vibrate around equilibrium positions.

Many hybrid organic-inorganic materials are messy. Examples include: 1) fullerene-based superatomic crystals (SACs), which have rotational degrees of freedom, 2) nanocrystal arrays (NCAs), whose building blocks are not atomically precise, and 3) self-assembled monolayers (SAMs), where weak bonding leads to large atomic displacements.

Thermal transport in these materials cannot be fully described in terms of phonons, precluding the rigorous application of lattice-dynamics based methods. Instead, molecular dynamics simulations can provide valuable insight into the nature of thermal transport and aid in interpreting experimental measurements.

In this tutorial, I will describe my group's work to model thermal transport in SACs, NCAs, and SAMs. I will cover how to build the structures, how to predict their thermal transport properties, and how to probe the atomic dynamics to discover the mechanisms of thermal transport. I encourage the tutorial participants to bring examples of messy system from their own research for additional discussion.

Biography:

Alan McGaughey is the Trustee Professor of Mechanical Engineering at Carnegie Mellon University with a courtesy appointment in Materials Science & Engineering. He holds B.Eng., M.A.Sc., and Ph.D. degrees in mechanical engineering from McMaster University, the University of Toronto, and the University of Michigan. His research group has been supported by NSF, DOE, AFOSR, ARO, and DARPA. He is a fellow of the ASME and the APS. He won the Air Force Office of Scientific Research Young Investigator Program award, was a Harrington Faculty Fellow at the University of Texas at Austin, and won the Teare Teaching Award at CMU. He has been voted "Professor of the Year" by the CMU mechanical engineering senior class three times. He has given invited talks and seminars on modeling atomistic transport across the United States and in Canada, Chile, China, France, Japan, Korea, and Singapore.