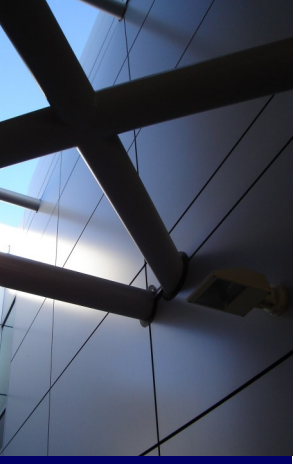

MECHANICAL ENGINEERING
DISSERTATION DEFENSE

The Department of Mechanical Engineering presents:

The Ph.D. Dissertation Defense of

Seyed Aria Hosseini

Thursday, May 27, 2021,
9am Pacific time

Prediction of Thermal and Electrical Transport in Nanostructured Materials for Energy Conversion Applications

Doctor of Philosophy, Graduate Program in Mechanical Engineering
University of California, Riverside, May 2021
Dr. Alex P. Greaney, Chairperson

Thermoelectrics (TE) are a class of materials that convert heat directly into electricity. If made sufficiently efficient and inexpensive, these materials could be used to recapture low-grade waste heat from the industrial process as useful electrical energy. The potential energy savings are vast. Recent studies by Lawrence Livermore National Laboratory have reported that more than 68% of U.S. energy consumption escapes as waste heat while recuperating *only* 10% of heat lost into electricity can improve fuel energy efficiency by 20%. This research presented here pursues strategies to make energy harvesting more efficient by using nanoengineering to improve the energy performance of TEs. Three significant theoretical insights are developed that together create a new design paradigm for engineering both thermal and electrical properties of TEs. The first strategy is to enhance the TE power factor through selectively filtering low-energy electrons. A *publicly-available* python design platform called *thermoelectric.py* with innovative mathematical approaches to accurately and efficiently compute, from first principles, the strength, and energy dependence of electron scattering from nanoscale pores and particles with different geometries is developed. The second strategy is the design of the nanoscale morphology of porous TEs to detriment the lattice thermal conductivity through phonon coherent effects. An analytical framework is laid out to model heat current anticorrelation (HCAC) in materials containing specific porous topologies. The model predicts that HCAC leads to an extreme reduction in thermal conductivity of up to 80% compared to structures in which the anticorrelation effect is not observed. The third strategy is a large-scale screening of TE alloys containing nanoscale porosity to find the minimum thermal conductivity. A general model is developed to predict lattice thermal conductivity of dielectrics containing nanoscale to macroscale porosity. The model is robust in providing a good approximation of the results from full Boltzmann transport (BTE) simulations of lattice thermal conductivity for a wide range of pores shapes, sizes, and spacings that span both the diffusive and ballistic regimes. This provides a simple yet accurate estimation of thermal transport in nanostructures that can be used to rapidly screen or design materials for a particular thermal task. As such this work provides an important tool to facilitate the design and discovery of materials for thermal-related applications, without explicitly solving the BTE.