

Quest for New Thermoelectric Materials: Theory and Computation Guided Discovery and Design

by Dr. Vladan Stevanović

Date: 1st July 2019 (Monday)

Time: 2.00pm – 3.00pm

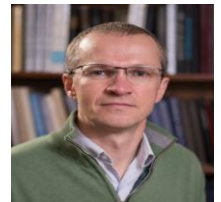
Venue: EA-06-04

Abstract

Progress in the widespread adoption of all solid heat-to-electricity technologies has largely been hindered by the absence of suitable thermoelectric materials. In pursuit for new thermoelectrics recent advances in large-scale deployment of first-principles calculations are increasingly being used in identifying new promising material systems. However, the need to predict electron and phonon transport properties with sufficient accuracy renders direct assessment of the thermoelectric figure of merit (zT) for large number of systems unfeasible. This forces computational searches to adopt approximations such as the constant relaxation time or constant mean free path that, by construction, cannot produce accurate ranking of materials. In this talk I will discuss our integrated theory-computation-experiment efforts in developing a robust set of material descriptors that: (1) are rooted in Boltzmann transport theory, but do not rely on largely inapplicable constant relaxation time or constant mean free path approximations, (2) are computationally tractable allowing material searches across large chemical spaces, and (3) are sufficiently accurate to provide reliable predictions. Our approach is demonstrated to correctly identify known thermoelectric materials and reliably suggest new and promising ones. I will review successes and failures in our quest for new thermoelectrics, extensions of our approach to quasi low-dimensional systems, and finally, discuss dopability as the critical outstanding challenge in achieving high zT materials.

Speaker

Vladan Stevanović is a theoretical solid-state physicist with multidisciplinary research background in applied, computational physics and materials science. He earned his Ph.D. degree from the Swiss Federal Institute of Technology, Lausanne and currently holds an Assistant Professor position in the Department of Metallurgical and Materials Engineering, Colorado School of Mines with the joint appointment at the National Renewable Energy Laboratory (NREL), both located in Colorado, USA. In pursuit for novel functional materials Vladan's research stands at the intersection between solid-state physics, materials science, large-scale (high-throughput) computations and big data. With the focus on renewable energy technologies, Vladan's research combines development and application of predictive methods to model relevant properties of real materials.



ALL ARE WELCOME!

Host: Prof Gong Hao