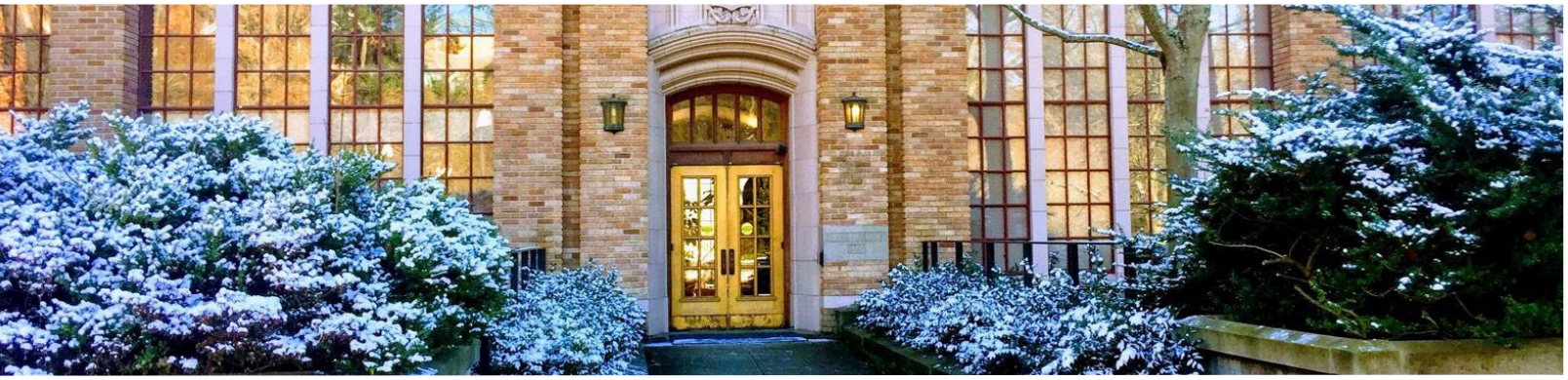
MSE 520: SEMINAR SERIES

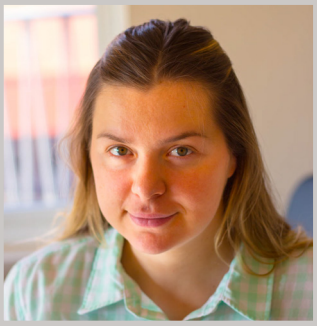
MATERIALS SCIENCE & ENGINEERING | SPRING 2018

APRIL 30, 2018 | 131 BAGLEY HALL | 3:30 PM



Thermodynamics And Transport Of Strongly Anharmonic Systems: A First-Principles Perspective

Phonons, or vibrational quanta of the atomic lattice, play an essential role in the thermodynamics, phase transitions, and transport of heat in solids. First-principles computational methods have provided unprecedented detail of these phenomena in weakly anharmonic solids but generally fail for materials with large nonlinearities. In this talk, I will describe a method based on the construction of effective Hamiltonians that accurate describes lattice dynamics in highly anharmonic solids. I will show how this approach allows us to resolve long-standing puzzles, including the effect of strong anharmonicity on high temperature phase stability, non-trivial temperature dependence of thermal resistivity of PbSe and the intrinsic upper bounds of lattice thermal conductivity in molecular solids.



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Nina Shulumba is a postdoctoral fellow in the Division of Engineering and Applied Science at Caltech. She received her B.S in 2009 and M.S. (summa cum laude) in 2011 in Theoretical Physics from St.Petersburg Polytechnic University in Russia. She conducted part of her M.S. research at the Ioffe Institute and she completed Ph.D. in Materials Science at Linköping University in Sweden in 2015, developing a new method for calculating the temperature dependent vibrational contribution to the free energy of a random alloy that accounts for anharmonicity. Her current research is focused on ab-initio modeling of transport phenomena in complex, anharmonic crystals.

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UNIVERSITY of WASHINGTON