

LA-SIGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Fall Seminar Series

3:30pm - 4:30pm, Wednesday, November 7, 2012

Johnston Hall, Room 338

Transport in Thermoelectric Materials

by

David J. Singh

Oak Ridge National Laboratory, Oak Ridge, TN



Abstract: There is increasing interest in thermoelectric materials motivated in part by recent progress and in part by the potential of these materials in various energy technologies. Thermoelectric performance is a multiply contra-indicated property of matter. For example, it requires (1) high thermopower and high electrical conductivity, (2) high electrical conductivity and low thermal conductivity and (3) low thermal conductivity and high melting point. The keys to progress are finding an optimal balance and finding ways of using complex electronic and phononic structures to avoid the counter-indications mentioned above. In this talk, I discuss some of the issues involved in the context of recent results. These include the surprising doping dependence of the thermopower in PbTe and PbSe, and the interplay between acoustic and optical phonons in PbTe. The potential of some new materials is discussed.

This work was done in collaboration with David Parker, Olivier Delaire and Mao-Hua Du and was supported by the Department of Energy through the S3TEC Energy Frontier Research Center.

Biography: David Singh is a Corporate Fellow at Oak Ridge National Laboratory where he is group leader for the Advanced Materials Group. He specializes in first principles calculations applied to functional materials including thermoelectrics, superconductors, ferroelectrics and radiation detection materials. He is a fellow of the American Physical Society. He obtained his Ph.D. Degree in Physics from the University of Ottawa, did postdoctoral work at the College of William and Mary and the Naval Research Laboratory, where he became a staff member serving until 2004. He has published a book on the LAPW method and more than 400 scientific papers.

