MM 24: Transport II: Thermal and Electrical Conductivity

Time: Tuesday 11:45–12:45 Location: H 0107

MM 24.1 Tue 11:45 H 0107

Thermal conductivity of half-Heusler thermoelectric materials from first principles — •Lars Bergqvist — Dept. of Materials and Nano Physics, KTH Royal Institute of Technology, Electrum 229, SE-164 40 Kista, Sweden — Swedish e-Science Research Centre (SeRC), KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Thermal conductivity and finite temperature phonon properties of half-Heusler thermoelectric materials are presented using large-scale ab-initio molecular dynamics simulations for calculation of interatomic force constants (IFC), including temperature and anharmonic effects, together with the full solution of the Boltzmann transport equation for phonons, as implemented in the newly developed Temperature Dependent anharmonic Effective Potential (TDEP) methodology.

Calculated lattice thermal conductivity, important for thermoelectric performance, show good agreement with experimental data. In particular, it is found that n-type ZrNiSn has lower conductivity than p-doped ZrCoSb, which can be analyzed in terms of the phonon lifetimes and broadening of the spectra from the dynamic structure factor at finite temperatures. Moreover, doping with Hf in ZrNiSn further reduces the thermal conductivity.

MM 24.2 Tue 12:00 H 0107

Microscopic theory and ab initio simulation of atomic heat transport — •Aris Marcolongo[1], Stefano Baroni[2], and Paolo Umari[3] — [1]Ecole Polytechnique Federale de Lausanne, Switzerland — [2]SISSA – International School for Advanced Studies, Trieste, Italy — [3]Department of Physics and Astronomy, Padua University, Italy

Green Kubo formulas, combined with classical molecular dynamics, are often used to compute thermal conductivity coefficients of liquid systems. Nevertheless, application to ab-initio molecular dynamics is often believed to be problematic because a suitable quantum-mechanical definition of the heat current is not readily available, due to the ill-definedness of the microscopic energy density to which it is related by the continuity equation. We argue that a similar difficulty actually exists in classical mechanics as well and show that it is nevertheless possible to obtain a physically well defined transport coefficient, independent of the ill defined microscopic energy density. We then derive an expliticit expression for the adiabatic energy current within density-functional theory, well defined under periodic boundary conditions. The resulting methodology is demonstrated by comparing ab initio and classical molecular simulations of a model liquid-Argon system, for which accurate inter-atomic potentials are derived by the force-matching method.

MM 24.3 Tue 12:15 H 0107

Topological insulators defined by local and non-local resistivity — •C. Shekhar[1], S. Ouardi[1], C. E. ViolBarbosa[1], B. Yan[1,2], W. Schnelle[1], G. H. Fecher[1], and C. Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Max Planck Institute for Physics of the Complex Systems, 01187 Dresden, Germany

Topological insulators are known for their metallic surface states, a result of strong spin-orbit coupling, that exhibit unique surface transport phenomenon. However, these surface transport phenomena are buried in the presence of metallic bulk conduction. We synthesized very high quality Bi_2 Te_2 Se single crystals by using a modified Bridgman method that possess high bulk resistivity of >20 Omega cm below 20K, whereas the bulk is mostly inactive and surface transport dominates. The temperature dependence of resistivity follows an activation law like a gap semiconductor in temperature range 20-300K. To define the topological property i.e. extract the surface transport from that of the bulk, we designed a special measurement geometry to measure the resistance in local and non-local regions. We find that single-crystal Bi_2 Te_2 Se exhibits a crossover from bulk to surface conduction at 20K. Simultaneously, the material also shows strong evidence of surface transport in magneto-conductance. This novel simple geometry facilitates finding evidence of surface transport in topological insulators, which are promising materials for future spintronic applications.

MM 24.4 Tue 12:30 H 0107

crystal growth, resistivity and hall effect of the delafossite metal PtCoO2 — pallavi kushwaha[1], philip moll[2], •nabhanila nandi[1], and andrew mackenzie[1,3] — [1]1 Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straβe 40, 01217 Dresden, Germany — [2]Laboratory for Solid State Physics, ETH Zurich, Switzerland — [3]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

We report single crystal growth of the delafossite oxide PtCoO2, and basic transport measurements on single crystals etched to well-defined geometries using focused ion beam techniques. The room temperature resistivity is 2.1 $\mu\Omega$cm, and the Hall coefficient is consistent with the existence of one free electron per Pt. Although the residual resistivity ratio is greater than fifty, a slight upturn of resistivity is seen below 15 K. The angle dependence of the in-plane magnetoresistance is also reported.