MM 40: Transport III - thermal transport

Time: Wednesday 10:15–11:15 Location: IFW D

MM 40.1 Wed 10:15 IFW D

TUNING QUANTUM ELECTRON AND PHONON TRANSPORT IN 2D MATERIALS BY STRAIN ENGINEERING: A GREEN'S FUNCTION BASED STUDY — •Leonardo Medrano Sandonas[1,2], Rafael Gutierrez[1], Alessandro Pecchia[3], Gotthard Seifert[4], and Gianaurelio Cuniberti[1,5,6] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Consiglio Nazionale delle Ricerche, Rome, Italy — [4]Institut für Physikalische Chemie und Elektrochemie, Dresden,Germany — [5]Dresden Center for Computational Materials Science, Dresden, Germany — [6]Center for Advancing Electronics Dresden, Dresden, Germany

In the present work, using a DFTB method in combination with Green's function approaches, we address strain engineering of the transport setup (contact-device(scattering)-contact regions) on the electron and phonon transport properties of 2D materials, focusing on hBN, phosphorene, and MoS_2 monolayer. Considering unstretched contact regions, we show that the electronic bandgap displays an anomalous behavior and the thermal conductance continuously decreases after increasing the strain level in the scattering region. However, when the whole system (contact and device regions) is homogeneously strained, the bandgap for hBN and MoS_2 monolayers decreases, while for phosphorene first increases and then tends to zero with larger strain levels. Additionally, the thermal conductance shows a specific strain dependence for each of the studied 2D materials.

MM 40.2 Wed 10:30 IFW D

***Ab initio* investigation of the anomalous phonon softening in FeSi** — •Robin Stern[1] and Georg K. H. Madsen[2] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]Institute of Materials Chemistry, TU Wien, Austria

The anomalous softening of the acoustic phonon peak in FeSi has recently received considerable experimental attention. In our work, we investigate the effect of thermal disorder on the lattice dynamics and the filling of the narrow band gap of FeSi using density functional theory. We show, by comparing the phonon density of states from temperature-independent and temperature-dependent force constants, that thermal structural disorder together with thermal expansion explains the anomalously strong renormalization of the acoustic phonons. Furthermore, we find an intricate interplay between thermal disorder and volume in gap closure.

MM 40.3 Wed 10:45 IFW D

Point defect phonon scattering and thermal conductivity in Silicon — •Bonny Dongre and Georg K. H. Madsen — Institute of Materials Chemistry, TU Wien, Getreidemarkt 9/165, 1060 Wien, Austria

Due to the ever decreasing size of devices and increasing operating speeds, understanding and control of the thermal transport has gained paramount importance. Predicting the thermal conductivity of such devices is an inherent multi-scale problem. This requires full description of thermal transport behavior on electronic level, atomistic and mesoscopic structure levels.

The aim of the present work is to systematically analyze the effect of various types of defects, e.g. vacancies, interfaces and dislocations inevitably present in engineering materials, on their thermal conductivities. When viewed from the atomistic scale, quantitative description of phonon scattering strength can be obtained using inputs from ab intio methods like DFT. We have used the atomic-green's-function approach to calculate the scattering rates which are then fed into the Boltzmann transport equation to get the required thermal conductivity in Vacancy Si (Vac_{Si}) and Germanium substitutional (Ge_{Si}) defect systems.

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MM 40.4 Wed 11:00 IFW D

Topological nodal line Dirac semimetal HfSiS — •Chandra Shekhar, Nitesh Kumar, Kaustuv Manna, Yanpeng Qi, Shu-Chun Wu, Binghai Yan, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Topological semimetals provide a wide platform to realize Dirac, nodal Dirac and Weyl fermions. Recently, HfSiS has been predicted as a nodal line Dirac semimetal. This compound shows hole carrier density which is higher as compare to the other known semimetals at 2K and massive amplitude of de Haas-van Alphen and Shubnikov-de Haas oscillations up to 30 K in 7 T. Low effective mass of the charge carriers acquire extra -Berry phase, a witness of topological Dirac type dispersion of bands which are originated from Si square net and Zr atoms. Furthermore, we establish the 3D Fermi-surface that consists of water caltrop-like electron and barley seed-like hole pockets. Asymmetrical nature of pockets is accountable to anisotropic magnetoresistance in HfSiS.