MM 39: Computational Materials Modelling - Transport, Excitations, Time Dependence I

Time: Wednesday 15:00–16:15 Location: H24

MM 39.1 Wed 15:00 H24

Thermal conductivity of graphene from first principles — •Andrea Cepellotti[1], Nicola Bonini[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Department of Physics, King's College London, London WC2R 2LS, United Kingdom

The thermal conductivity of graphene is computed from the Boltzmann equation for phonon transport, where phonons are treated semiclassically and vibrational properties and anharmonic scattering rates are obtained from density-functional perturbation theory. We show that the commonly used single-mode relaxation time approximation (SMRTA) is not accurate, even at high temperatures, due to the unusually large number of normal scattering processes compared to umklapp ones. By relaxing the SMRTA and solving the Boltzmann equation self-consistently [1] we are able to recover excellent agreement with experimental data [2]. We also rationalize the variations in experimental measurements as an effect of sample finite dimensions, due to the large contributions coming from long wavelength phonons. As pointed out in previous simulations [3], we underline the critical role of strain in the renormalization of the out-of-plane acoustic modes and quantify its effects. Finally, we show how strain and sample size can be used to tune thermal conductivity in graphene over a large range of values.

[1] M. Omini and A. Sparavigna, Nuovo Cimento D **19**, 1537 (1997).
[2] A. A. Balandin, Nat. Mater. **10**, 569 (2011).
[3] N. Bonini, J. Garg and N. Marzari, Nano Lett. **12**, 2673 (2012).

MM 39.2 Wed 15:15 H24

High Temperature Thermal Conductivity from First Principles — •Christian Carbogno[1], Rampi Ramprasad[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs

In spite of significant research efforts, a first principles determination of the thermal conductivity at high temperatures has remained elusive. Under such conditions, techniques that rely on the harmonic approximation are no longer valid, while standard non-equilibrium molecular dynamics methods require huge temperature gradients that lead to deviations from Fourier's law. The Green-Kubo method [1], which does not suffer from these shortcomings, involves the assessment of the thermal conductivity from the auto-correlation of the heat flux in equilibrium. In classical MD, the heat flux is computed from the energetic contributions of the individual atoms; we show that the Green-Kubo approach can be reformulated in terms of the energy and stress densities [2], which are directly accessible in DFT calculations. This approach leads to a unique definition of the heat flux that does not rely on any partitioning scheme for the total energy. We critically discuss the computational cost, the accuracy, and the applicability of this approach by investigating the thermal conductivity for oxides and semiconductors with low thermal conductivities.

[1] R. Kubo, M. Yokota, S. Nakajima, J. Phys. Soc. Jpn. 12, 1203 (1957).
[2] R. Ramprasad, J. Phys. Condens. Matter 14, 5497 (2002).

MM 39.3 Wed 15:30 H24

Ab-initio study of q-dependent screening parameters and effective plasma frequencies in simple metals — •Steffen Kaltenborn and Hans Christian Schneider — University of Kaiserslautern, 67653 Kaiserslautern, Germany

We present results of an ab-initio study of the dielectric function $\varepsilon(\mathbf{q},\omega)$ in the RPA approximation together with energies and wave functions from density functional theory [1,2]. We have implemented the linear tetrahedron method for the computation of the dielectric function and therefore do not need to use a phenomenological broadening of the energy conserving delta function. From the dielectric function we determine the effective plasma frequency Ω and the static screening wave number κ for the simple metals aluminum, silver and copper. In all metals, we find a pronounced deviation from the parabolic dispersion $\Omega \propto q^2$ of the plasma frequency that is often assumed [3]. In particular, for aluminum the effective plasma frequency decreases with finite **q**-vectors until it reaches the electron-pair continuum. We also discuss the influence of the spin mixing on plasma frequency and screening wave number. Last, we compare our results with measurements [4] and with computed results using a finite broadening in the RPA dielectric function, as implemented in current DFT codes [1,2].

[1] DFT-Program Elk FP-LAPW Code, http://elk.sourceforge.net.
[2] C. Ambrosch-Draxl et al., Comp. Phys. Commun. 175, 1-14, (2006).
[3] G. Piazza et al., Solid State Commun. 51, 905-908, (1984).
[4] Ellen J. Zeman et al., J. Phys. Chem. 91, 634-643 (1987).

MM 39.4 Wed 15:45 H24

Spectral density and metal-insulator phase transition in Mott insulators within RDMFT — •Sangeeta Sharma, John Kay Dewhurst, and E. K. U. Gross — Max-Planck-Institut for Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We present a method for calculating the spectrum of periodic solids within reduced density matrix functional theory. This method is validated by a detailed comparison of the angular momentum projected spectral density with that of well established many-body techniques, in all cases finding an excellent agreement. The physics behind the pressure induced insulator-metal phase transition in MnO is investigated. The driving mechanism of this transition is identified as increased crystal field splitting with pressure, resulting in a charge redistribution between the Mn eg and t2g symmetry projected states.

MM 39.5 Wed 16:00 H24

Embedded impurity method applied to positron annihilation lifetime simulations — •Martin Offenberger[1], John Banhart[2], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universität München — [2]Helmholtz-Zentrum Berlin für Materialien und Energie

Within the Korringa-Kohn-Rostoker (KKR) framework of solid state simulations, the embedded impurity method is an efficient alternative to the supercell ansatz to describe impurity systems like substituted atoms or vacancies. This approach allows to study electronic properties and interactions between different alloying elements and vacancies on an atomic level.

As positrons are strongly attracted to vacancies and to a lesser degree to certain types of impurities, this method is of great advantage for positron annihilation studies.

We demonstrate the implementation of structural relaxation around impurities into the Munich SPRKKR band structure program package. Corresponding results for positron annihilation lifetimes of impurity-vacancy cluster systems embedded into Aluminium will be presented.

In addition the potential models (ASA or full potential) used within KKR calculations and their influence on electron and positron calculations for embedded impurity systems will be discussed.