MM 76: Methods in Computational Materials Modelling (methodological aspecst, numerics)

Heat Transport

Time: Friday 11:15–12:30 Location: TC 006

MM 76.1 Fri 11:15 TC 006

Non-equilibrium dynamics of quantum heat transport in nanoscale devices — •Leonardo Medrano Sandonas[1,2], Alexander Croy[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1,3,4] — [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]Dresden Center for Computational Materials Science, Dresden, Germany — [4]Center for Advancing Electronics Dresden, Dresden, Germany

Next to electrons, phonons play a major role for the behavior of nanoscale devices. Additionally, phononics and nano-mechanics offer the possibility to steer and manipulate phonons. Hence, a more detailed understanding of phonon dynamics is required. Using an auxiliary-mode approach, which has successfully been applied for the case of electrons [1], we present a method to describe time-dependent phonon transport based on the time evolution of the phonon density matrix. We compute the phonon density matrix by employing the non-equilibrium Green*s function formalism. This method allows us to gain insight into the behavior of local vibrations which are driven by time-dependent temperature differences between heat reservoirs [2,3]. In the present work, we apply this methodology to study the time dependence of the thermal current in molecular junctions. [1] B. S. Popescu and A. Croy, New J. Phys. 18, 093044, (2016). [2] R. Tuovinen et al., Phys. Rev. B 93, 214301, (2016). [3] Marcone I. Sena-Junior et al., J. Phys. A: Math. Theor. 50, 435202, (2017)

MM 76.2 Fri 11:30 TC 006

Anharmonic Effects in Solids: Putting Third-Order Expansion to the Test — •Florian Knoop, Hagen-Henrik Kowalski, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The standard *ab initio* formalism to compute thermal conductivities of solids relies on determining the second and third order force constants of the zero Kelvin potential-energy surface [1]. To understand the role of higher-order contributions not accounted for in such an approach, we investigate the thermal conductivities of a series of materials with increasing anharmonicity (e. g. Si, Ga_2O_3, CsCl, ZrO_2) using two advanced methodologies: Temperature-dependent effective potentials, in which higher-order anharmonicity is incorporated by a renormalization of lower-order force constants via statistical finite-temperature sampling [2] and the *ab initio* Green-Kubo formalism, in which all anharmonic effects are assessed non-perturbatively through *ab initio* molecular dynamics simulations [3]. We describe the computational challenges, e. g., finite time and size effects and the choice of the exchange-correlation functional. Eventually, we discuss how the obtained quantitative thermal conductivities allow for a qualitative understanding of high-order anharmonic nuclear dynamics and the implications for other vibrational properties of real materials.
[1] D. A. Broido, *et al.*, *Appl. Phys. Lett.* **91**, 231922 (2007).
[2] O. Hellman and I. A. Abrikosov, *Phys. Rev. B* **88**, 144301 (2013).
[3] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

MM 76.3 Fri 11:45 TC 006

Generalized Langevin Thermostats for Tuning Dynamical Properties in Quantum Dynamics — •Mariana Rossi[1], Venkat Kapil[2], and Michele Ceriotti[2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]EPFL, Switzerland

Generalized Langevin Equation (GLE) thermostats have been used very effectively as a tool to manipulate and optimize the sampling of thermodynamic ensembles and the associated static properties. Here [1] we show that a similar, exquisite level of control can be achieved for the dynamical properties computed from thermostatted trajectories. By developing quantitative measures of the disturbance induced by the GLE to the Hamiltonian dynamics of a harmonic oscillator, we show that these analytical results accurately predict the behavior of strongly anharmonic systems.We address the use of thermostats in the context of approximate path-integral-based models of quantum nuclear dynamics, demonstrating that a custom-tailored GLE can alleviate some of the artifacts associated with these techniques, improving the quality of results for the modelling of vibrational dynamics of molecules, liquids and solids. Finally we show the power of this technique by showing the importance of nuclear quantum effects in the close to full suppression of NH stretch signals in porphyrin derivatives.
[1] M. Rossi, V. Kapil, M. Ceriotti, JCP **148**, 102301 (2018)

MM 76.4 Fri 12:00 TC 006

Molecular Dynamics Simulation of Periodic Nanostructuring of Au due to UV Laser Pulse under Water Layer on the Experimental Scale — •Dmitry Ivanov[1,2], Andreas Blumenstein[2,3], Baerbel Rethfeld[2], Juergen Ihlemman[3], Peter Simon[3], and Martin Garcia[1] — [1]Physics Department, University of Kassel, 34132 Kassel, Germany — [2]Physics Department, Technical University of Kaiserslautern and OPTIMAS Research Centre, 67663 Kaiserslautern, Germany — [3]Laser-Laboratorium Göttingen e.V., 37033 Göttingen, Germany

The physical mechanism of materials surface restructuring involves a lot of fast, non-equilibrium, and interrelated processes while the solid is in a transient state. While the experimental investigation of the material restructuring mechanism can be limited to post-priory observations, the theoretical methods, working within a single computational approach with corresponding spatial and temporal scales, cannot address all physical aspects of the nanostructuring process. In this work we propose a combined atomistic-continuum approach suitable for the investigation of periodic nanostructuring mechanism due to a UV ultrashort laser pulse on the experimental scale. The combined model is applied to investigate the nanostructuring mechanism under conditions of vacuum ambient and in the regime of spatial confinement due to a thick water layer above the target. The obtained results, generated on the same temporal and spatial scales as they are in the experiment, allowed to extract the main mechanisms of nanostructuring process and the reasons for a higher quality of structures generated under water.

MM 76.5 Fri 12:15 TC 006

Resistor network simulation method for graphene-based conductive fibers — •Leo Rizzi[1,4], Andreas Zienert[2], Jörg Schuster[3], and Martin Köhne[4] — [1]Faculty of Electrical Engineering and Information Technology, Technische Universität Chemnitz, Chemnitz, Germany — [2]Center for Microtechnologies (ZfM), Technische Universität Chemnitz, Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [4]Robert Bosch GmbH, Stuttgart, Germany

In recent years, graphene fibers (GFs) have emerged as a new form of electrical conductors. They consist of an assembly of graphene sheets spun into a textile fiber. GFs are lightweight, mechanically strong, and corrosion resistant. Defect-engineering and doping strategies have continuously improved the electrical conductivity of fibers towards metallic levels. However, it still remains below the conductivities of silver or copper.
While several groups have presented experimental results on the production of GFs, theoretical descriptions predicting their electrical behavior are less advanced. We present a simulative approach to model the electrical conductivity of GFs, based on a three-dimensional random network of resistors. We investigate the influence of the raw material's properties on the fiber electrical conductivity and identify the main influence parameters. Our results offer a deeper understanding of GFs and can be helpful to further enhance their electrical performance.