O 52: Focus Session: Electron-Phonon Interactions I

Organizers: Lilia Boeri (Sapienza, Rome, Italy) and Claudia Draxl (Humboldt-Universität zu Berlin)

Time: Wednesday 10:30–12:45 Location: H15

Invited Talk O 52.1 Wed 10:30 H15

Electron-boson coupling in correlated materials: a non-equilibrium perspective — •Claudio Giannetti[1], Stefano Dal Conte[2], Giulio Cerullo[2], and Andrea Damascelli[3] — [1]ILAMP, Università Cattolica del Sacro Cuore, via Musei 41, 25121 Brescia, Italy — [2]Department of Physics, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy — [3]Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada

Non-equilibrium techniques are emerging as a unique tool to investigate the coupling of electrons to bosonic degrees of freedom in correlated materials. The recent advances in ultrafast science have paved the way to the study of electron-phonon and electron-spin interactions on their relevant timescales (10-100 fs).

In this talk we will provide an overview of the recent advances in the field and we will discuss the energy relaxation process in conventional anisotropic superconductors and in strongly-correlated materials, with particular focus on superconducting copper oxides.

O 52.2 Wed 11:00 H15

Electron-phonon coupling in laser-induced nonequilibrium states of solids — Tobias Held[1], Sebastian T. Weber[1], Isabel Klett[1], Jan Vorberger[2], and •Baerbel Rethfeld[1] — [1]Fachbereich Physik und Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern — [2]Institut für Strahlenphysik, Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden

Ultrafast laser pulses heat electrons in solids to highly nonequilibrium distributions. The subsequent energy transfer to the lattice induce nonequilibrium distributions in the phonon system as well. We analyse, how these nonequilibrium states influence the electron-phonon energy transfer as compared to the standard two-temperature model.

Motivated by a nonthermal lattice model [1], we determine the energy transfer from the hot electrons to different phonon modes. The partial Eliashberg functions are obtained with DFT methods, while the relaxation dynamics is traced with help of Boltzmann collision integrals. We also evaluate phonon-phonon scattering terms and examine the phonon relaxation and its influence on the electron-phonon energy transfer [2]. Finally, we show that the electron-phonon scattering can induce a secondary nonequilibrium state in the electron distribution persisting on the timescale of lattice heating [3].

[1] L. Waldecker, R. Bertoni, R. Ernstorfer, J. Vorberger, PRX 6, 021003 (2016).
[2] I. Klett and B. Rethfeld, PRB 98, 144306 (2018).
[3] S.T. Weber and B. Rethfeld, arXiv:1801.06560 (2018).

O 52.3 Wed 11:15 H15

A real space view on the complex renormalization of quasiparticles mediated by electron-phonon interactions — •Jon Lafuente-Bartolome[1,2], Peio Garcia-Goiricelaya[1,2], Idoia G. Gurtubay[1,2], and Asier Eiguren[1,2] — [1]Materia Kondentsatuaren Fisika Saila, University of the Basque Country UPV/EHU, 48080 Bilbao, Basque Country, Spain. — [2]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, 20018 Donostia-San Sebastián, Spain.

We present a novel numerical approach to resolve the real space details of renormalized quasiparticle states and their accompanying virtual phonon cloud in interacting electron-phonon systems. The analytical continuation of the momentum dependent electron self-energy onto the complex-energy plane is performed, where multiple quasiparticle solutions of the Dyson equation can be found. Our method improves previous procedures by overcoming the particle-hole symmetry approximation, and is readily applicable to realistic systems of current interest such as monolayer MoS_2, for which we show some illustrative results.

O 52.4 Wed 11:30 H15

Temperature-dependent optical spectra and band structures using the *ZG*-configuration — •Marios Zacharias and Feliciano Giustino — Department of Materials, University of Oxford, Oxford

Typical calculations of the optoelectronic properties of solids are performed by describing the nuclei as classical particles clamped to their crystallographic positions. This approximation inevitably misses the quantum zero-point motion and thermal effects, as well as phonon-assisted optical processes [1]. Recently we developed a new methodology to incorporate these effects in electronic structure calculations by describing the electron-phonon interaction via the Zacharias-Giustino (*ZG*)-configuration [2]. In this talk I will show the theory behind this *one-shot* method, and I will demonstrate how it can be derived rigorously from the Williams-Lax theory of temperature-dependent electronic transitions [3] in conjunction with the harmonic approximation. I will discuss some recent examples of calculations that have been performed using the *ZG*-configuration, including temperature-dependent band structures and optical spectra of indirect and direct band gap semiconductors. This method holds promise for high-throughput calculations of any property at finite temperature that can be described by the Fermi's Golden rule.

[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).
[2] M. Zacharias, and F. Giustino, *Phys. Rev. B* **89**, 075125 (2016).
[3] M. Zacharias, C. E. Patrick, and F. Giustino, *Phys. Rev. Lett.* **115**, 177401 (2015).

Invited Talk O 52.5 Wed 11:45 H15

Carrier lifetime trends in highly efficient thermoelectrics — •Vidvuds Ozolins — Yale University

Recent developments in electronic structure algorithms based on the Wannier function interpolation of electronic wave functions have enabled accurate first-principles calculations of electron-phonon interactions and intrinsic carrier lifetimes in the relaxation time approximation. This has supplied the final missing piece of the puzzle for predicting the thermoelectric figure of merit $zT = \frac{\sigma S^2 T}{\kappa}$, where the conducrtivity σ, the Seebeck coefficient S, and the total thermal conductivity κ now can all be obtained from the density-functional theory (DFT). This opens up exciting possibilities for theoretically understanding and reliably predicting new materials with high values of zT. We will review several examples from our recent work, including a Li-intercalated analogue of lead telluride (Li_2TlBi), an intermetallic compound with unexpectedly high value of S (CoSi), and a theoretically predicted full Heusler compound with ultrahigh zT (Ba_2BiAu). General factors for high thermoelectric power factors in these compounds include energy dependence of carrier lifetimes for high S, high degeneracy of carrier pockets at the Fermi level, weak electron-phonon scattering for high mobility, and concomitantly low Lorentz numbers for low electronic thermal conductivity.

O 52.6 Wed 12:15 H15

Thermally-Enhanced Fröhlich Coupling in SnSe — •Fabio Caruso, Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin

To gain insight into the peculiar temperature dependence of the thermoelectric material SnSe, we employ many-body perturbation theory and explore the influence of the electron-phonon interaction on its electronic and transport properties. We show that a lattice dynamics characterized by soft highly-polar phonons induces a large thermal enhancement of the Fröhlich interaction. We account for these phenomena in ab-initio calculations of the photoemission spectrum and electrical conductivity at finite temperature, unraveling the mechanisms behind recent experimental data. Our results reveal a complex interplay between lattice thermal expansion and Fröhlich coupling, providing a new rationale for the in-silico prediction of transport coefficients of high-performance thermoelectrics.

O 52.7 Wed 12:30 H15

Fully-Anharmonic, First-Principles Theory of Electronic Transport — •Zhenkun Yuan, Marios Zacharias, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Under typical operation conditions, thermoelectric charge and heat transport are limited by scattering events resulting from electron-

phonon coupling (EPC). Although much progress has been made in assessing the respective electronic transport coefficients in the harmonic approximation [1], recent evidence suggests that anharmonic contributions both in the nuclear motion ***and*** the EPCs can play a decisive whereas typically ignored role [2]. We here present a first-principles formalism that fully accounts for these anharmonic effects in electronic transport: Anharmonicity in the nuclear motion is accounted for via *ab initio* molecular dynamics, while anharmonicity in the EPCs is included by evaluating the electronic self-energy along these trajectories in a real-time density-matrix formalism. This gives access to the electronic charge and heat fluxes, enabling us to obtain the thermoelectric transport coefficients via the fluctuation-dissipation theorem. Using both harmonic elemental semiconductors and anharmonic perovskites as example, we discuss the advantages and challenges of the proposed approach.