TT 7: SC: Properties, Electronic Structure, Mechanisms 2

Time: Monday 14:00–16:15 Location: HSZ 301

TT 7.1 Mon 14:00 HSZ 301

Importance of spin-orbit coupling for the electron-phonon interaction of the strong-coupling superconductor Pb — •Rolf Heid[1], Klaus-Peter Bohnen[1], Irina Sklyadneva[2,1], and Evgeni Chulkov[2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik — [2]Donostia International Physics Center, San Sebastian, Spain

Electron-phonon coupling (EPC) properties can nowadays be calculated routinely from first principles within a DFT-based linear-response approach. All previous studies, however, have been carried out in a semi-relativistic framework, which does not take into account the effects of spin-orbit coupling (SOC). Based on a recent implementation of the SOC for linear response calculations within a mixed-basis pseudopotential approach [1], we analyze the effect of SOC on the EPC for the prototype strong-coupling superconductor Pb. We find that SOC increases the coupling constant λ by 44%, solving the longstanding puzzle of too small λ values obtained consistently in previous first principles calculations. The origin of the SOC-induced enhancement of λ lies both in a softening of the phonon spectrum and in an increase of the EPC matrix elements, which significantly improves the agreement with tunneling experiments. We also find a large influence of SOC on phonon-induced electronic self-energies and lifetimes. Finally, consequences for EPC properties of thin Pb films will be discussed.
[1] R. Heid, K.-P. Bohnen, I. Yu. Sklyadneva, E. V. Chulkov, Phys. Rev. B **81**, 174527 (2010)

TT 7.2 Mon 14:15 HSZ 301

First principles study of the spin-orbit coupling effect on the Tl-Pb-Bi superconducting alloys — •Omar De la Peña-Seaman, Rolf Heid, and Klaus-Peter Bohnen — Karlsruher Institut für Technologie (KIT), Institut für Festkörperphysik, Germany

We have studied the influence of spin-orbit coupling (SOC) on the phonon properties, the electron-phonon (e-ph) coupling and on the superconducting properties for the Pb-Bi and Pb-Tl alloys in the stable fcc-phase doping regimes. These systems have been studied within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloys. The Eliashberg spectral function ($\alpha^2F(\omega)$) and the electron-phonon coupling parameter (λ) have been calculated with and without SOC. The observed effects of SOC in the full phonon dispersion and $\alpha^2F(\omega)$ consist in a softening of the phonon frequencies and an increase of the e-ph coupling matrix elements, which become weaker on the Tl-rich side. SOC enhances λ by as much as 48% in some cases and improves its overall behavior as a function of the concentrations for the alloy systems, leading to a very nice agreement with experimental data from tunneling measurements.

TT 7.3 Mon 14:30 HSZ 301

Effects of the Born-Oppenheimer approximation in the electronic band structure of MgB_2 and ZrB_2. — •Vivien Petzold and Helge Rosner — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

Electronic band structure calculations are routinely applied to many problems in chemistry and physics. The methods rely on a number of approximations, where the treatment of exchange and correlation is a very prominent issue, probably the most prominent in the development of new density functionals in the framework of density functional theory (DFT). The present work highlights effects that arise from the more fundamental Born-Oppenheimer approximation. Based on this approximation, the original problem - the quantum-mechanical description of matter consisting of nuclei and electrons - is decomposed into a nuclear and an electronic problem, the latter of which is treated by electronic band structure methods. Utilizing the most common density functionals, the local density approximation (LDA) and the generalized gradient approximation (GGA), we observe deviations between experimental and theoretical de Haas van Alphen (dHvA) frequencies for MgB_2 and ZrB_2 that can be consistently understood by electron-phonon coupling effects, which the theory is lacking. The explanation is based on a highly accurate computation of dHvA frequencies indicating an electron-phonon coupling-induced shift of the electronic bands.

TT 7.4 Mon 14:45 HSZ 301

Vibrational and thermal properties of ternary semiconductors and their isotopic dependence: chalcopyrite $CuGaS_2$ — •Reinhard K. Kremer[1], Manuel Cardona[1], Rudolf Lauck[1], Aldo H. Romero[2], and Alfonso Munoz[3] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]CINVESTAV, Unidad Queretaro, Queretaro, Mexico — [3]MALTA Consolider Team, Dep. de Fisica, Universidad de La Laguna, La Laguna , Tenerife, Spain

The availability of ab initio electronic calculations and the concomitant techniques for deriving the corresponding lattice dynamics have been profusely used in the past decade for calculating thermodynamic and vibrational properties of semiconductors, as well as their dependence on isotopic masses. The latter have been compared with experimental data for elemental and binary semiconductors with different isotopic compositions[1]. Here we present experimental and theoretical data for several vibronic and thermodynamic properties of a canonical ternary semiconductor of the chalcopyrite family: $CuGaS_2$[2]. Among these properties are the lattice parameters, the phonon dispersion relations and densities of states (projected on the Cu, Ga, and S constituents), the specific heat and the volume expansion coefficient. The calculations were performed with the ABINIT and VASP codes within the LDA approximation for exchange and correlation.
[1] M. Cardona, et al., PRB 81, 075202 (2010).
[2] Gibin et al., Solid State Commun 133, 569 (2005); Sanati et al. Solid State Commun. 131 229 (2004).

TT 7.5 Mon 15:00 HSZ 301

Fermi-surface topology of the $Ce_{1-x}Yb_xCoIn_5$ — •A. Polyakov[1], O. Ignatchik[1], A. D. Bianchi[2], B. Prevost[2], G. Seyfarth[2], Z. Fisk[3], D. Hurt[3], R. G. Goodrich[4], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), FZ Dresden-Rossendorf, Germany — [2]Department of Physics, University of Montreal, Canada — [3]Department of Physics and Astronomy, University of California, USA — [4]Department of Physics, George Washington University, USA

The heavy-fermion (HF) metals are very susceptible to chemical substitution. In these compounds the Kondo coupling between a lattice of local moments and the conduction band creates quasiparticle excitations with large effective masses and the dopants disrupt the coherent Kondo coupling. We study the effect of Yb doping on the Pauli-limited, HF superconductor, $CeCoIn_5$ via de Haas-van Alphen (dHvA) measurements. Yb acts as a non-magnetic divalent substitution for Ce, equivalent to hole doping on the rare-earth site. Our main goal consists in the systematic investigation of the dHvA oscillations on $Ce_{1-x}Yb_xCoIn_5$ in order to elucidate the evolution of the Fermi surface as a function of Yb. The dHvA data were obtained on high-quality single crystals with different concentrations of Yb atoms. The experiment was performed in a top-loading dilution refrigerator by use of a capacitive torque cantilever technique at temperatures down to 20 mK in magnetic fields up to 18 T.

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TT 7.6 Mon 15:15 HSZ 301

Order parameter in $CeCu_2Si_2$ — •Hugo A. Vieyra[1], Manuel Brando[1], Niels Oeschler[1], Silvia Seiro[1], Hirale S. Jeevan[2], Christoph Geibel[1], David Parker[3], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden 01187, Germany — [2]I. Physik. Institut, Georg-August-Universität Göttingen, Göttingen 37077, Germany — [3]US Naval Research Laboratory. Washington, DC 20375, USA

Understanding the interplay between magnetism and unconventional superconductivity remains a key challenge in solid-state physics. A clear example is the archetypical heavy-fermion compound $CeCu_2Si_2$ which exhibits superconductivity (T_c=600 mK) in the vicinity of a magnetic quantum critical point. It is believed that magnetic fluctuations mediate superconductivity and its order parameter possesses d-wave symmetry, both ideas still under debate. In this work, a high-quality single crystal with a purely superconducting ground state (S type) has been chosen to investigate the low-temperature thermal- and electric-transport characteristics of the superconducting state. Non-vanishing contributions of low-energy quasiparticle excitations to the thermal transport ($\kappa_0/T > 0$) suggest the presence of nodal structure

in $CeCu_2Si_2$. In turn, angle-dependent resistivity measurements of the upper critical field H_{c2} point towards unconventional superconductivity with d-wave symmetry of the order parameter. Theoretical calculations reveal the strong influence of Pauli paramagnetic effects and a d_{xy} symmetry of the gap function.

TT 7.7 Mon 15:30 HSZ 301

Spin fluctuation mediated Cooper-pairing in non-centrosymmetric $CePt_3Si$ — •Ludwig Klam[1] and Dirk Manske[2] — [1]Institut für Theoretische Physik, Wolfgang-Pauli-Str. 27, CH-8093 Zürich — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart

Non-centrosymmetric superconductors, and in particular $CePt_3Si$, attract special interest, since the antisymmetric spin-orbit coupling provides the unique opportunity to consider a microscopic mixture of a spin singlet and triplet superconducting order parameter. An efficient numerical method is introduced in order to calculate the dynamical spin and charge response of $CePt_3Si$, using an itinerant description for the electrons. With a realistic parametrization of the band structure, the nesting function is calculated for a selected band in the normal non-magnetic state. From the spin and charge susceptibility, a superconducting pairing interaction is constructed for the weak-coupling gap equation. A sign analysis of the decoupled gap equation supports the experimental evidence of a strong triplet contribution to the order parameter in $CePt_3Si$. In particular for this compound, it can be shown that an increasing Rashba-type of spin-orbit coupling strengthens the triplet contribution.

TT 7.8 Mon 15:45 HSZ 301

Electronic properties of molecular picene — •M. Grobosch[1], F. Roth[1], B. Mahns[1], M. Gatti[2], P. Cudazzo[2], B. Büchner[1], A. Rubio[2], and M. Knupfer[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]Nano-Bio Spectrocopy Group and ETSF Scientific Development Centre, Dpto. Física de Materiales Universidad del País Vasco, Av. Tolosa, E-20018 San Sebastían, Spian

We have studied the electronic properties of molecular picene by a combination of accurate experimental (photoemission spectroscopy, absorption spectroscopy) and theoretical spectroscopy to get a deeper insight into the occupied and unoccupied electronic states of this recently discovered organic semiconductor. By means of combined photoelectron spectroscopy (XPS, UPS) we have determined the ionization potential of solid picene to be 6.4 eV and a work function of 4.4 eV, i.e. picene is rather stable against oxidation. The first occupied electronic levels of picene are quite close in energy and the onset of the electronic DOS is at about 2 eV below the chemical potential indicating a quite large band gap of solid picene. The C1s excitation data of solid picene measured using EELS compared to the unoccupied electronic DOS calculated in the GW approximation are in very good agreement if GW corrections are taken into account.

TT 7.9 Mon 16:00 HSZ 301

Dynamic response and anomalous plasmon dispersion of potassium doped picene — •Friedrich Roth[1], Benjamin Mahns[1], Mandy Grobosch[1], Matteo Gatti[2], Pierluigi Cudazzo[2], Bernd Büchner[1], Angel Rubio[2], and Martin Knupfer[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Nano-Bio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, Av. Tolosa 72, E-20018 San Sebastián, Spain

We performed electron energy-loss spectroscopy studies in order to get a deeper insight into the electronic structure of the potassium intercalated picene and the peculiar physical properties of this recently discovered superconductor. A comparison of the loss function of the undoped and doped compound shows the appearance of a new peak in the optical gap, which we attributed to a charge carrier plasmon. We find a remarkable negative plasmon dispersion and a dramatic increase for the value of the background dielectric constant ϵ_∞ upon doping.