TT 36: Superconductivity: Properties, Electronic Structure, Order Parameter

Time: Friday 10:15–13:00 Location: H 0104

TT 36.1 Fri 10:15 H 0104

Electron-Phonon interaction in electron-doped graphites — •Lilia Boeri[1], Ole Krogh Andersen[1], Jun Sung Kim[1], Reinhard Kremer[1], Giovanni B. Bachelet[2], and Matteo Giantomassi[3] — [1]Max-Planck-Institut für FestkörperForschung, Stuttgart, Germany — [2]INFM SMC and Dipartimento di Fisica, Università "la Sapienza", Roma, Italy — [3]UPCM, Université Catholique de Louvain, Louvain-la-Neuve,Belgium

The discovery of superconductivity in MgB_2 has initiated a thorough search for new electron-phonon ($e-ph$) superconductors, particulary among hexagonal layered compounds.

In this talk I will describe, using *ab-initio* methods, the electron-phonon properties of two classes of recently discovered superconductors, namely alkali-earth intercalated graphites (highest T_c 15.1 K for CaC_6)and metal-intercalated ternary compounds of the form: MaAlSi (highest T_c=7.8 K for CaAlSi).

TT 36.2 Fri 10:30 H 0104

Anisotropic s-wave superconductivity in graphite intercalation compounds: CaC_6 and SrC_6 — •Jun Sung Kim[1], Lilia Boeri[1], Feridoon Razavi[2], and Reinhard Kremer[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraβe 1, D-70569 Stuttgart, Germany — [2]Department of Physics, Brock University, St. Catharines, Ontario, L2S 3A1, Canada

We have investigated the anisotropy of the superconducting properties for newly-discovered superconducting graphite intercalation compounds, CaC_6 and SrC_6 using specific heat (C_p). The electronic C_p for CaC_6 shows an exponential temperature dependence at low temperatures, consistent with a fully gapped s-wave superconducting order parameter. However, the detailed comparison with an isotropic superconducting gap model shows significant deviation between experiment and theory. From the magnetic field dependence of C_p, the anisotropy of upper critical fields (H_{c2}) for CaC_6 is ~ 5, consistent with that obtained from the magnetic field dependence of Sommerfeld coefficient, but much larger than that of SrC_6. In comparison with electronic structure calculations, we found that the isotropic gap model cannot explain observed superconducting properties, suggesting significant anisotropy in the superconducting gap for both CaC_6 and SrC_6. Recent investigations on a directional point-contact spectroscopy on CaC_6 along the c-axis and ab-plane will also be discussed.

TT 36.3 Fri 10:45 H 0104

Superconducting properties of CaC_6 — •Antonio Sanna[1,2], Gianni Profeta[3], Andrea Floris[2], Andrea Marini[4], Eberhard K.U. Gross[2], and Sandro Massidda[1] — [1]Università degli studi di Cagliari, Italy. — [2]Freie Universität Berlin, Germany. — [3]Università degli studi dell'Aquila, Italy. — [4]University of Rome Tor Vergata, Italy.

We present first-principles calculations of the superconducting properties of CaC_6[1], obtained within the density functional theory of superconductivity (SCDFT). We find an anisotropic gap which is larger on the Fermi surface sheet with interlayer character. In contrast to MgB_2 the intraband anisotropy is large and the gaps on the three Fermi surface sheets overlap. The resulting critical temperature of 9.5 K is in good agreement with the experimental value of 11.5 K.

We show that anisotropy improves the agreement between calculated and experimental specific heat and is consistent with tunnelling experiments. A direct evidence of the gap anisotropy in CaC_6 has been recently observed in directional point contact measurements[2].

We also investigate the system under pressure in order to analyse the increase of the superconducting critical temperature reported experimentally[3] but not reproduced in the McMillan approach. Within our SCDFT implementation we intend to improve the theoretical description with respect to previous studies introducing an ab-initio and pressure-dependent Coulomb interaction.

[1] A. Sanna *et al.*, Phys. Rev. B **75**, 020511 (2007).
[2] R. Gonnelli *et al.*, arXiv 0708.0921.
[3] A. Gauzzi *et al.*, Phys. Rev. Lett. **98**, 067002 (2007).

TT 36.4 Fri 11:00 H 0104

High-pressure study of layered bulk phases of elemental boron — •Jens Kunstmann[1], Lilia Boeri[1], and Jens Kortus[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Inst. für Theoretische Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg, Germany

The valence shell of boron contains less electrons than available orbitals, which results in very complex bulk structures, primarily consisting of B_{12} icosahedra. But boron is relatively little studied and many properties such as the phase diagram, the ground state structure, and its high-pressure behavior are unknown. Recently two discoveries put elemental boron into the scientific focus. One is that it becomes superconducting under high pressure. The other one is that small clusters form two-dimensional sheet-like structures, as suggested by theoretical studies of Boustani and Quandt in the mid-1990s. The high-pressure superconductivity is not fully understood so far, because the corresponding crystal structures are still under debate. Hence before solving the problem of understanding the coupling mechanism for superconductivity one has to solve first the problem of determining the crystal structure. The existence of sheet-like clusters poses the question if boron sheets, similar to graphene, or layered bulk phases, similar to graphite, may also exist for boron. Therefore our study tries to approach the following questions: What do such layered bulk structures look like? What are their stabilities in comparison with other bulk phases? Are they dynamically stable and if yes, are they responsible for the high-pressure superconductivity of elemental boron?

TT 36.5 Fri 11:15 H 0104

Electrons, phonons and superconducting properties of CaBeSi — •A. Floris[1], C. Bersier[1], A. Sanna[1,2], G. Profeta[3], A. Continenza[3], E.K.U. Gross[1], and S. Massidda[2] — [1]Institut für Theoretische Physik, Freie Universität Berlin, Germany — [2]INFM SLACS and Dipartimento di Scienze Fisiche, Università degli Studi di Cagliari, Italy — [3]C.A.S.T.I. - INFM and Dipartimento di Fisica, Università degli studi dell'Aquila, Italy

We present first-principles calculations on the normal and superconducting state of $CaBe_xSi_{2-x}$ $(x = 1)$[1,2], in the framework of the density functional theory for superconductors (SCDFT)[3,4] . CaBeSi is isostructural and isoelectronic to MgB_2 and this makes possible a direct comparison of the electronic and vibrational properties and the electron-phonon interaction of the two materials. Although our calculations show that CaBeSi has a low critical temperature ($T_c \approx 0.6$ K), it exhibits a complex gap structure, with *three* gaps at the Fermi level. Besides the two σ and π gaps, present also in MgB_2, the appearance of a third gap is related to the anisotropy of the Coulomb repulsion, acting in different way on the bonding and antibonding electronic π states.

[1] N. May *et al.*, Z. Naturforsh. B **2**, 1947 (1977).
[2] F. Sano *et al.*, CP850 Low Temperature Physics: 24^{th} International Conference on Low Temperature Physics, 2006.
[3] M. Lüders *et al.*, Phys. Rev. B, **72**, 024545 (2005).
[4] M. A. L. Marques *et al.*, Phys. Rev. B, **72**, 024546 (2005).

15 min. break

TT 36.6 Fri 11:45 H 0104

Superconductivity in the new filled skutterudites $M\mathbf{Pt_4Ge_{12}}$ (M = La, Pr, Sr, Ba) — •Walter Schnelle, Roman Gumeniuk, Helge Rosner, Michael Nicklas, Andreas Leithe-Jasper, and Yuri Grin — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

New germanium-platinum compounds with the filled-skutterudite crystal structure were synthesized [1]. The crystal structure and composition were investigated by X-ray diffraction and microprobe analysis. Magnetic susceptibility, specific heat, and electrical resistivity measurements evidence superconductivity in $LaPt_4Ge_{12}$ and $PrPt_4Ge_{12}$ below 8.3 K. The parameters of the normal and superconducting states were established. Strong coupling and a crystal electric field singlet groundstate is found for the Pr compound. Electronic structure calculations show a large density of states at the Fermi level [1]. Similar behavior albeit with lower T_c was observed for $SrPt_4Ge_{12}$ and $BaPt_4Ge_{12}$ [1,2].

[1] R. Gumeniuk *et al.* Phys. Rev. Lett. submitted. ArXiV 0710.1413v1.
[2] R. Gumeniuk *et al.* Poster, this conference.

TT 36.7 Fri 12:00 H 0104

Eliashberg Theory of Superconductivity and Inelastic Scattering by Rare-Earth Impurities in the Filled Skutterudite $La_{1-x}Pr_xOs_4Sb_{12}$ — •Jun Chang[1], Ilya Eremin[1,2], Peter Thalmeier[3], and Peter Fulde[1] — [1]Max-Planck Institut fur Physik komplexer Systeme, D-01187 Dresden, Germany — [2]Institute fur Mathematische und Theoretische Physik, TU-Braunschweig, D-38106 Braunschweig, Germany — [3]Max-Planck Institut fur Chemische Physik fester Stoffe, D-01187 Dresden, Germany

We study the influence of inelastic rare-earth impurity scattering on electron-phonon mediated superconductivity and mass renormalization in $(La_{1-x}Pr_x)Os_4Sb_{12}$ compounds. Solving the strong coupling Eliashberg equations we find that the dominant quadrupolar component of the inelastic scattering on Pr impurities yields an enhancement of the superconducting transition temperature T_c in $LaOs_4Sb_{12}$ and increases monotonically as a function of Pr concentration. The calculated results are in good agreement with the experimentally observed $T_c(x)$ dependence. Our analysis suggests that phonons and quadrupolar excitations cause the attractive electron interaction which results in the formation of Cooper pairs and singlet superconductivity in $PrOs_4Sb_{12}$.

TT 36.8 Fri 12:15 H 0104

Evidence for an Fulde-Ferrell-Larkin-Ovchinnikov state in a layered organic superconductor — •B. Bergk[1], P. H. M. Böttger[1], R. Lortz[2], Y. Wang[2], A. Demuer[3], I. Sheikin[3], G. Zwicknagl[4], Y. Nakazawa[5], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, FZ Dresden-Rossendorf, 01314 Dresden, Germany — [2]Department of Condensed Matter Physics, University of Geneva, CH-1211 Geneva, Switzerland — [3]Grenoble High Magnetic Field Laboratory, CNRS, 38042 Grenoble, France — [4]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [5]Department of Chemistry, Osaka University, 1-1, Machikaneyama, Toyonaka, Osaka, Japan

We present specific heat and torque-magnetization data of the layered organic superconductor κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ in high magnetic fields up to 28 T and at low temperatures down to 1.5 K. The magnetic field was aligned perfectly parallel to the superconducting planes of the sample. In that orientation and at low temperatures the upper critical field, B_{c2}, gets close to the Pauli limit which is about 21 T. But instead of the expected saturation at this field value we observe an upturn of B_{c2} towards low temperatures. This comes along with a change of the order of the phase transition from second order to first order. In addition, another first-order phase transition appears below B_{c2} in the superconducting state. These features strongly point to the formation of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase in the state above the Pauli limit. Our results are in line with the behaviour predicted for FFLO states in two-dimensional systems.

TT 36.9 Fri 12:30 H 0104

Electron Phonon Interaction and Superconductivity in Nb and Pb investigated with Neutron Resonance Spin Echo Spectroscopy — •Pegor Aynajian[1], Thomas Keller[1,2], Lilia Boeri[1], Klaus Habicht[3], and Bernhard Keimer[1] — [1]Max-Planck-Institut für Festkrperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]ZWE FRMII, TUM, Lichtenbergstrasse 1, D-85748 Garching, Germany — [3]3Hahn-Meitner-Institut, Glienicker Strasse 100, D-14109 Berlin, Germany

The momentum and temperature dependency of the phonon lifetime of the transverse acoustic branches along the [110] and [100] directions in Pb and Nb were studied using the high resolution neutron resonance spin-echo, triple-axis technique. Several anomalies were observed, which can in part be assigned to Kohn anomalies. The most striking feature both in Nb and Pb is a Kohn anomaly sitting at a phonon energy corresponding to the superconducting energy gap 2D(T = 0). This arises the question if 2D is limited by a Kohn anomaly.

TT 36.10 Fri 12:45 H 0104

Localized superconductivity in TiN thin films — •Ante Bilušić[1], Tatyana Baturina[2], Tatyana Mironov[2], Florian Otto[1], Mikhaïl Baklanov[3], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, Germany — [2]Institute of Semiconductor Physics, Novosibirsk, Russia — [3]IMEC, Leuven, Belgium

We present a low-temperature investigation of transport and magnetic properties of TiN thin films in the critical region of the disorder driven superconductor-insulator transition (SIT). At zero magnetic field, the superconducting and insulating phases are sharply separated, indicating the absence of the intermediate metallic state in the SIT. Electrical conductivity of the insulating films is thermally activated. Films closer to the critical level of disorder show a huge positive magnetoresistance (MR) at low, and a negative MR for high fields. Films being deeper on the insulating side of the SIT critical region exhibit negative MR only. At low temperatures, differential conductance curves of insulating samples show a depinning threshold V_T, below which the conductance is immeasurably small. Threshold V_T depends in a nonmonotonic way on magnetic field. This can be explained in terms of recent theory [1], which relies on the competition of Coulomb charging and Josephson coupling in arrays of Josephson junctions.

[1] M. V. Fistul, V. M. Vinokur, and T. I. Baturina, arXiv:0708.2334v2 (unpublished)