MM 51: Electronic Properties I

Time: Thursday 10:15–11:15 Location: H5

MM 51.1 Thu 10:15 H5

Momentum resolved Eliashberg function calculations within the KKR formalism — •Sergiy Mankovsky, Jan Minar, and Hubert Ebert — Dept. Chemie und Biochemie/Phys. Chemie, Universität München, Butenandtstr. 11, D-81377, München, Germany

We present an expression for the calculation of the momentum resolved Eliaschberg function $\alpha^2F(\omega,\vec{k})$ within the KKR Green's function formalism. All underlying calculations of the electron-phonon matrix elements as well as of the phonon energies are based on ab-initio electronic structure calculations performed using the fully relativistic spin-polarised KKR band structure method. Applications have been done for various non-magnetic as well as for magnetic systems. The Eliaschberg function obtained within these calculations have been used to evaluate the electron-phonon self-energy $\Sigma_{\vec{k}}$. The self-energies obtained are compared with those obtained from angle resolved photoemission spectroscopy (ARPES). In all cases studied so far a very satisfying agreement was achieved.

MM 51.2 Thu 10:30 H5

First-principles electronic structure and chemical bonding studies of type I clathrates $Ba_8T_xE_{46-x}$ (T: late transition metals; E: Si, Ge; $x = 0$–6) — •Alim Ormeci, Umut Aydemir, Wilder Carrillo-Cabrera, Michael Baitinger, and Yuri Grin — Max Planck Institute for Chemical Physics of Solids, Dresden

In recent years type I clathrates doped with transition metals have attracted a lot interest largely due to the expectations that such materials may have interesting electronic and transport properties. The cubic unit cell of type I clathrates contains two 20- and six 24-framework atom cages. The voids enclosed by these cages can be filled with alkali, alkaline-earth or rare earth metals, while transition metals or Ga can substitute some of the framework atoms yielding three-component compounds. Here, the interest is confined to Si or Ge as main framework atoms, Ba as filler, and some late transition metals selected from Groups 9-12 as dopants. The dopants usually occupy the 6c Wyckoff position (space group $Pm\bar{3}n$, no. 223), however the range of 6c site occupation fraction depends on the dopant and the framework atom, Si or Ge. Vacancies at 6c sites are a possibility and observed mostly in Ge clathrates rather than in Si ones. Using the full-potential local orbital (FPLO) method and supercells containing up to 216 atoms, electronic structures, chemical bonding and heats of formation will be investigated for the systems $Ba_8T_xE_{46-x}$ with E: Si, Ge and for $x =$ 0–6 allowing also for the possibility of vacancies, as well. Theoretical results will be compared with experimental findings.

MM 51.3 Thu 10:45 H5

Optical and electrical characterization of Al doped Zinc oxide nanoporous films prepared via sol-gel method — •Babak Nasr, Subho Dasgupta, Robert Kruk, and Horst Hahn — Karlsruhe Institute of Technology (KIT) GmbH,Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Highly transparent and conducting ZnO films doped with different Al concentration prepared via sol-gel method. In this study one of the most important deposition parameters, heat ramping at pre-heat-treatment step, was investigated to grow high porous thin films in high surface area applications. It was found that high porosity is obtainable by fast heat ramping of the gel films. In addition the optical and electrical properties of Al doped ZnO films as a function of carrier concentration was studied using UV-Vis, FTIR spectroscopy, and four points measurement. The films were all transparent in visible range and had a sharp absorption around 380 nm. A blue shifts of the absorption edge respect to undoped ZnO has been observed as a function of the carrier concentration up to 2 at.% Al doping due to Burstein-Moss effect. Strongly resonance absorption at plasma frequency in near infra red region led to calculation of carrier concentration. These investigations were complemented by photoconductivity measurement to understand the impact of surface states in electronic structure of the films. Among different doped films with atomic ratio of 0.5 to 4 with increments of 0.5 the systems with 1.5at.% to 2at.% show the lowest resistivity and widest optical band gap.

MM 51.4 Thu 11:00 H5

Positronic structure in metals containing vacancies — •Martin Offenberger[1], Hubert Ebert[1], and John Banhart[2] — [1]Ludwig-Maximilians-Universität München — [2]Helmholtz Zentrum Berlin

Positron anihilation is a well established tool to study defects in metals. Corresponding theoretical calculations for the positronic structure for such systems are made so far using standard band structure codes together with the so-called super cell approach. We present a fully relativistic approach that makes use of multipe scattering theory, i.e. the Korringa-Kohn-Rostoker Green's function (KKR-GF) method, to avoid artificial boundary conditions. This is achieved by dealing with the defect region by means of the Dyson equation. First results will be presented for the density of states and charge distributions for a positron captured by a vacancy in various metals as Al, Cu and Fe. The change of these properties due to adjacent impurities will be discussed in addition.