

MM 14: Electronic Properties I

Time: Monday 16:45–18:30

Location: H 0111

MM 14.1 Mon 16:45 H 0111

Band structure mapping and calculations of metallic MoTe₂ — •THORSTEN ZANDT, ROBERT HEIMBURGER, CHRISTOPH JANOWITZ, and RECARDO MANZKE — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

Calculations of the electronic structure have been performed using an self-consistent full potential linearized augmented-plane-wave (FP-LAPW) method in order to compare MoTe₂ in its two metallic forms, i. e. β - and Td-MoTe₂. In β - and Td-MoTe₂ the metal atom is displaced from the centre of an octahedron of Te atoms, and metal-metal chains with bond lengths only slightly longer than in the elemental metals occur along the layers. Thus one can guess that β - and Td-MoTe₂ are normal metals. From the band structure calculations we found that only few bands cross the Fermi energy. In the total DOS this leads to a distinct minimum at the Fermi energy. Therefore our interpretation is that MoTe₂ forms semimetals rather than metals, which is in good agreement with observed low conductivity [1]. The electronic structure between the monoclinic α -phase and orthorhombic β -phase of MoTe₂ is essentially unchanged. We discuss the theoretical results in comparison with experimental valence band studies using angle-resolved photoelectron spectroscopy taken from measurements at BESSY II.

[1] T. Zandt, H.Dwelk, C. Janowitz, and R. Manzke, *Journal of Alloys and Compounds*, 442, 216-218 (2007)

MM 14.2 Mon 17:00 H 0111

Spectral-weight analysis from ellipsometric spectroscopy on FeSi single crystals — •DIRK MENZEL¹, PAUL POPOVICH², ALEXANDER BORIS², ANA MARIA RACU¹, and JOACHIM SCHOENES¹ — ¹TU Braunschweig, Institut für Physik der Kondensierten Materie — ²Max-Planck-Institut für Festkörperforschung, Stuttgart

One of the key arguments of the supporters of the description of FeSi as Kondo insulator stems from reflectivity measurements. After Kramers-Kronig analysis (KKR) of these data the resulting optical conductivity spectra in some cases [1] show a loss of spectral weight when the gap opens at low temperature, which is not recovered in the neighborhood of the gap, while in some cases it does not [2]. Since the determination of absolute conductivity values from reflectivity spectra is problematic, we have undertaken ellipsometry measurements from the far-infrared to the UV spectral range, giving directly - without KKR - the optical conductivity. We find that the spectral weight is not compensated up to 2.5 eV. At low temperatures the indirect gap amounts to 33 meV and is filled at a temperature of about 250 K. This is in agreement with our recent Raman investigations indicating a change in the effective masses of the charge carriers as function of temperature which results in a shift of the chemical potential towards the valence band [3]. It is discussed if an interaction among *d*-electrons can be the origin of the widely spread spectral-weight recovery.

[1] Z. Schlesinger et al., *Phys. Rev. Lett.* **71**, 1748 (1993).

[2] L. Degiorgi et al., *Europhys. Lett.* **28**, 341 (1994).

[3] A. M. Racu et al., *Phys. Rev. B* **76**, 115103 (2007).

MM 14.3 Mon 17:15 H 0111

Parity of substrate bands probed by quantum-well states of overlayer — •DENIS VYALIKH¹, YURIY KUCHERENKO², FREDERIK SCHILLER³, MATTHIAS HOLDER¹, ANDREAS KADE¹, SERGUEI MOLODTSOV¹, and CLEMENS LAUBSCHAT¹ — ¹Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — ²Institute of Metal Physics, National Academy of Sciences of Ukraine, UA-03142 Kiev, Ukraine — ³Departamento de Fisica de Materiales, Universidad del Pais Vasco, E-20018 Spain

Quantum-well (QW) states in metallic nanostructures are objects of continued interest and exhibit permanently novel fascinating phenomena. In the present contribution we demonstrate by means of by angle-resolved photoelectron spectroscopy (ARPES) study of Ag/W(110) supported by Layer Korrington-Kohn-Rostoker (LKKR) calculations that energy overlap of QW and substrate bands of the same parity lead to the formation of broad hybridization gaps around the k-point of the crossings. Since the symmetry properties of two-dimensional QW bands can easily be determined, they can successfully be used as fingerprints to probe parity of substrate bands. The parity data provide information about site-specific localization of electron densities that may be used, e.g. to understand interactions in

correlated materials like high-temperature superconductors (electron-phonon coupling) or heavy-fermion systems (f-d hybridization). References: 1) D. V. Vyalikh et al., *Phys. Rev. B* **76**, 153406 (2007).

MM 14.4 Mon 17:30 H 0111

High Kinetic Energy Photoelectron Spectroscopy at BESSY — •MIHAELA GORGOI¹, SVANTE SVENSSON², MARCEL MERTIN¹, FRANZ SCHÄFERS¹, and WALTER BRAUN¹ — ¹BESSY GmbH, Berlin, Germany — ²Uppsala University, Uppsala, Sweden

The present work will show the investigation possibilities offered by the recently developed high kinetic energy photoelectron spectroscopy (HIKE) at the Berliner synchrotron light source. Hard x-ray photoemission has proven to be a non-destructive depth profiling tool for the characterisation of bulk electronic properties of different types of materials as well as interface properties of organic and inorganic thin films and multilayers. The HIKE end station operates at the KMC-1 bending magnet beamline. Electron spectra have been recorded using x-ray energies from 2 keV up to 12 keV excitation energies. Exemplifying results will be given in order to demonstrate the performance of the technique and its advantages.

MM 14.5 Mon 17:45 H 0111

Global exploration of the energy landscape of solids on the ab initio level — •KLAUS DOLL, J CHRISTIAN SCHÖN, and MARTIN JANSEN — Max-Planck-Institute for Solid State Research, D-70569 Stuttgart, Germany

Predicting which crystalline modifications can be present in a chemical system requires the global exploration of its energy landscape. Due to the large computational effort involved, in the past this search for sufficiently stable minima has been performed employing a variety of empirical potentials and cost functions followed by a local optimization on the ab initio level. However, this entails the risk of overlooking important modifications that are not modeled accurately using empirical potentials. In order to overcome this critical limitation, we develop an approach to employ ab initio energy functions during the global optimization phase of the structure prediction. As an example, we perform a global exploration of the landscapes of LiF [1] and BN on the ab initio level and show that the relevant crystalline modifications are found during the search.

[1] K. Doll, J. C. Schön and M. Jansen, *Phys. Chem. Chem. Phys.*, in press

MM 14.6 Mon 18:00 H 0111

Calculations of the force-constant tensor within the KKR Green's function method — •SERGIY MANKOVSKY and HUBERT EBERT — Dept. Chemie und Biochemie/Phys. Chemie, LMU München, Butenandtstr. 11, D-81377 München, Deutschland

We present a formalism for the calculation of the force-constant tensor within the KKR Green's function method. As a primary information the formalism gives the real-space force-constant tensor, i.e. the pairwise interaction parameters, on the basis of ab-initio electronic structure calculations. Accordingly, the technique is applicable in principle to any system as for example solids, surfaces and nanostructures. In addition this feature opens the way for a number of interesting applications. First results for the force-constant tensor of solid state systems will be presented together with corresponding results for the phonon dispersion relation. Comparison will be made with experiment and results of other theoretical works.

MM 14.7 Mon 18:15 H 0111

Residual resistance calculations of transition metal alloys including short-range ordering effects — •STEPHAN LOWITZER¹, DIEMO KÖDDERITZSCH¹, HUBERT EBERT¹, JULIE STAUNTON², and PAUL TULIP² — ¹Department Chemie und Biochemie, LMU München, Butenandtstr. 11, 81377 München — ²Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom

The residual resistance (at T = 0K) of Cu_xZn_{1-x} and Ag_xPd_{1-x} has been calculated. For these calculations the Kubo-Greenwood formalism has been employed. The electronic structure calculations are based on the fully relativistic Korrington-Kohn-Rostoker (KKR) band structure method in connection with the coherent potential approximation (CPA) alloy theory. To deal with short-range ordering effects we used

the more elaborated nonlocal coherent potential approximation (NL-CPA). Our results show the expected behavior of decreasing resistivity

when one includes short-range ordering effects in good agreement with experimental data.