MM 46: Electronic Properties II

Time: Thursday 16:45–18:00 Location: IFW B

MM 46.1 Thu 16:45 IFW B

The Korringa-Kohn-Rostoker method: its mathematical foundations — •Robert Hammerling — Center for Computational Materials Science, TU Wien, 1060 Wien — Wolfgang Pauli Institute, Uni Wien, 1090 Wien

The Korringa-Kohn-Rostoker(KKR) method is a well-established method in condensed matter physics to calculate the static Green function of a one-body Schrödinger operator. The multi-site problem is split in a single site problem and the evaluation of the free Green function under appropriate boundary conditions. While both ingredients individually are well understood the resulting expression for the multi-site Green function is still questioned in the mathematical physics community. In this work the mathematical foundations of the KKR method are critically examined.

MM 46.2 Thu 17:00 IFW B

Structural and magnetic properties of Fe under pressure — •Sergey Mankovsky, Jan Minar, Svitlana Polesya, and Hubert Ebert — Dept. Chemie und Biochemie/Phys. Chemie, Universität München, München, Deutschland

The structural bcc→hcp phase transition in Fe under pressure has been investigated on the basis of ab-initio electronic structure calculations using the KKR Green's function method. The role of the magnetic order on the stability of the bcc structure was studied. For this purpose an analysis of the total energy and magnetic structure was performed at different pressure values along a transformation path connecting the bcc and hcp structures. This allows an explanation of the small differences in pressure dependent structural and magnetic XAS signals observed experimentally. In addition, calculations of phonon spectra at different pressure values have been performed. They are based on the formalism of the calculation of the real-space force-constant tensor within the KKR Green's function method. An analysis of different contributions to the dynamical matrix shows the responsibility of the exchange splitting of spin-up and spin-down energy bands for the stabilisation of bcc structure at low pressure.

MM 46.3 Thu 17:15 IFW B

A theoretical description of spin resolved transport — •Stephan Lowitzer[1], Diemo Ködderitzsch[1], Hubert Ebert[1], and Julie B. Staunton[2] — [1]Department Chemie und Biochemie, LMU München, Butenandtstraße 11, 81377 München — [2]Department of Physics, University of Warwick, Coventry CV4 7AL, UK

Spin resolved transport became during the last years a fast growing field of interest for many theoretical working groups. We present an approximative scheme to calculate the spin decomposed conductivity within the Kubo-Greenwood formalism. The electronic structure calculations are based on the fully relativistic Korringa-Kohn-Rostoker (KKR) band structure method in connection with the coherent potential approximation (CPA) alloy theory. To demonstrate the reliability of our approach we apply this formalism to $Fe_{1-x}Cr_x$ and the diluted magnetic semiconductor system (DMS) $Ga_{1-x}Mn_xAs$.

MM 46.4 Thu 17:30 IFW B

First-principle study of the connection between structure and electronic properties of gallium — •Elena Voloshina[1], Krzysztof Rosciszewski[2], and Beate Paulus[1] — [1]Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, Germany — [2]Institute of Physics, Jagiellonian university, Reymonta 4, 30059 Krakow, Poland

Different structures of gallium have been studied by means of density functional theory (DFT). The density of states of orthorhombic α-Ga, the only elemental solid exhibiting both metallic and molecular character at zero pressure, shows a pseudogap at the Fermi energy. Complex analysis of the relation between lattice structure and the corresponding electronic properties allows us to throw a light upon an origin of the pseudogap. We have found that the free-electron-like behavior which is a property of the high-pressure *bct* and *fcc* phases of gallium depends strongly on the arrangement of atoms in the buckled planes, one of the building blocks of the orthorhombic gallium.

MM 46.5 Thu 17:45 IFW B

Quantum effects on the Elasticity of Graphene: An ab-initio and tight binding study — •Soumya Bera[1], Andreas Arnold[1], and Ferdinand Evers[1,2] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — [2]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76128 Karlsruhe, Germany

One of the most interesting aspect of single layer graphene is its surface corrugation (ripples), which can either be intrinsic or induced by surface roughness of the substrate. The long wavelength elastic properties of this novel material are also of great interest and we investigate them here. Our focus is on elasticity in the presence of ripples. We are going to employ two distinct methods namely ab-initio and tight binding calculations, in order to study the effect of ripples together with there associated zero modes on elasticity.

Our ab-initio study supports the exceptional quadratic dispersion relation of flexural(out-of-plane) phonons which is imposed by the spatial symmetries in the long wavelength limit of elastic theory. While short wavelength optical phonons have been studied in the past, to the best of our knowledge our work is the first ab-initio study on the long wave-length context. This DFT analysis also suggests a considerable amount($\sim 4\%$) of change in elastic constants due to zero point motion of phonons originated from the in-plane strain in the system. Using a tight binding model with nearest neighbor hopping we are now exploring the impact of zero energy states on elasticity. Here the source of these zero energy states is strain, induced by ripples.