DS 41: Layer Properties: Electrical, Optical, and Mechanical Properties II

Time: Thursday 15:00–16:45 Location: CHE 91

DS 41.1 Thu 15:00 CHE 91

Magnetoconductivity in ZnMnO thin films with anisotropic, highly conductive surface layers modelled by the Thouless diffusion length and valley degeneracy factor. — •Sahitya V. Vegesna[1], Danilo Bürger[1], Rajkumar Patra[1], Barbara Abendroth[2], Ilona Skorupa[1,3], Oliver G. Schmidt[1,4], and Heidemarie Schmidt[1] — [1]Material Systems for Nanoelectronics, Technische Universität Chemnitz, 09126 Chemnitz, Germany — [2]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Straße 23, 09596 Freiberg, Germany — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [4]Institute for Integrative Nanosciences, IFW Dresden, Dresden 01069, Germany.

Magnetoresistance (MR) of n-type ZnMnO thin films with Mn 5 at% on sapphire have been studied in in-plane and out-of-plane magnetic fields up to 6 T in the temperature range from 5 K to 300 K. Superimposed positive and negative MR model for ZnCoO thin films [1], has been extended in order to include a valley degeneracy factor which accounts for the formation of electronic levels close to the Fermi level of n-ZnMnO due to substitutional Mn ions and their effect on the negative MR in ZnMnO. MR has been modeled with s-d exchange of 0.2 eV and Mn electron spin (5/2) for single layer transport in two dimensions and for single layer transport in three dimensions and for two layer parallel transport in two and three dimensions. Modeled Thouless diffusion length is proportional to $T^{-0.5}$ [2]. [1]Q. Xu et al., Phys. Rev. B 76, (2007).[2]T. Andrearczyk et al., Phys. Rev. B 72, (2005).

DS 41.2 Thu 15:15 CHE 91

ZrO_2 as a high-k dielectric matrix for electrical applications - formation of embedded Ge nanocrystals and a Ta-stabilized orthorhombic phase — •David Lehninger[1], Julia Wünsche[1], Frank Schneider[1], Volker Klemm[2], Mykhaylo Motylenko[2], David Rafaja[2], and Johannes Heitmann[1] — [1]Institut für Angewandte Physik, TU Bergakademie Freiberg, D-09596 Freiberg — [2]Institut für Werkstoffwissenschaft, TU Bergakademie Freiberg, D-09596 Freiberg

Germanium nanocrystals (nc) embedded in dielectric matrices are discussed as absorbers for third generation solar cells, as sensitizers for rare earth elements, and as charge trapping layer for nonvolatile memories. Here, the formation of Ge nc in a $TaZrO_x$ matrix was studied. Single $GeTaZrO_x$ and $TaZrO_x$ layers as well as superlattices consisting of alternating $GeTaZrO_x$- and $TaZrO_x$-layers with different compositions were sputtered. Crystallization of Ge and $TaZrO_x$ was characterized by transmission electron microscopy, Raman scattering, and X-ray diffraction. It has been found that Ge nc with spherical shape and well-defined size embedded in amorphous $TaZrO_x$ can be formed. The superior properties of single layers of such Ge nc for charge trapping applications were already shown [1]. At elevated annealing temperatures the amorphous $TaZrO_x$ matrix crystallizes in a non-centrosymmetric orthorhombic phase. This makes this material system attractive for fully CMOS compatible ferroelectric applications. [1] D. Lehninger, P. Seidel, M. Geyer, F. Schneider, V. Klemm, D. Rafaja, J. von Borany, J. Heitmann, *Appl. Phys. Lett.* **106**, 023116 (2015)

DS 41.3 Thu 15:30 CHE 91

Controlling the Conductivity of Ti_3C_2 MXenes by Inductively Coupled Oxygen and Hydrogen Plasma Treatment and Humidity — •Florian M. Römer[1], Ulf Wiedwald[1], Tanja Strusch[1], Joseph Halim[2], Elisa Mayerberger[2], Michel W. Barsoum[2], and Michael Farle[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Department of Materials Engineering, LeBow Engineering Center 27-445, Drexel University, Philadelphia, PA 19104-2875, United States of America

Herein we report on the conductivity of plasma and humidty treated Ti_3C_2 MXene thin films of 13 nm thickness. The latter were produced by spincoating a colloidal solution, which was made by LiF/HCl etching of Ti_3AlC_2 powders. We exposed the films to oxygen and hydrogen plasma, measured the resistivity and investigated them by X-Ray photoelectron spectroscopy. We found that the metallic resistivities can be switched reproducibly by plasma treatment between 5.6$\mu\Omega$m (oxidized state) and 4.6$\mu\Omega$m (reduced state).

By removing the relative humidity from 80% down to ultra high vacuum conditions, we decreased the resistance from 6340Ω to 243Ω – a 26 fold reduction. This makes MXenes a possible candidate as high precision nano sized humidity and gas sensors.

DS 41.4 Thu 15:45 CHE 91

Competing order in the fermionic Hubbard model on the hexagonal graphene lattice — •Dominik Smith[1], Lorenz von Smekal[1], Pavel Buividovich[2], and Maksim Ulybyshev[2] — [1]Justus-Liebig-Universität, Gießen, Deutschland — [2]Universität Regensburg, Regensburg, Deutschland

We study the phase diagram of the fermionic Hubbard model on the hexagonal lattice in the space of on-site and nearest neighbor couplings with Hybrid-Monte-Carlo simulations. With pure on-site repulsion this allows to determine the critical coupling strength for spin-density wave formation with the standard approach of introducing a small mass term, explicitly breaking the sublattice symmetry. The analogous mass term for charge-density wave formation above a critical nearest-neighbor repulsion, on the other hand, would introduce a fermion sign problem. The competition between the two and the phase diagram in the space of the two coouplings can however be studied in simulations without explicit sublattice symmetry breaking. Our results compare qualitatively well with the Hartree-Fock phase diagram.

DS 41.5 Thu 16:00 CHE 91

Hybrid Monte-Carlo simulations at the van Hove singularity in mono-layer graphene — •Michael Körner, Dominik Smith, and Lorenz von Smekal — Institut für Theoretische Physik, Justus-Liebig-Universität Gießen

We use Hybrid Monte-Carlo (HMC) simulations to investigate the influence of long range electron-electron interactions on the electronic band structure of single layer graphene. Here we are particularly interested in the region where the fermi surface crosses the van Hove singularity, and where a topological electronic transition called a neck-disrupting Lifshitz transition occurs. We simulate with HMC a partially screened Coulomb potential and, due to the fermion sign problem, a spin-dependent chemical potential to study the influence of long range interactions on this topological transition in finite volumes and at non-vanishing temperatures. Our goal is to determine how interactions change the character of the topological transition and if there is a set of parameters for which a real phase transition in the thermodynamic sense can occur.

DS 41.6 Thu 16:15 CHE 91

The Phase Diagram of the hexagonal Hubbard Model with Dyson-Schwinger Equations — •Katja Kleeberg and Lorenz von Smekal — Institut für Theoretische Physik, Justus-Liebig Universität Gießen

We study the semimetal-insulator transition on the hexagonal lattice within the framework of Dyson-Schwinger equations. The coupled Dyson-Schwinger equations are formulated for the two competing phases, either realized by a charge-density wave formation or a spin-density wave formation. We investigate the critical behaviour for zero temperature within an extended Hubbard model with on-site and nearest-neighbour interaction. The critical coupling strengths are determined for an unscreened interaction (i.e. in Hartree-Fock approximation) and with static Lindhard screening included. The resulting phase diagrams for the fermionic Hubbard model are compared. The Dyson-Schwinger euqations are solved numerically by fixed-point iteration on GPU's for very large lattices which gives access to the study of the associated magnetic and finite-size scaling behaviour.

DS 41.7 Thu 16:30 CHE 91

Laser spectroscopic in-situ temperature measurements on surfaces — •Eugen Speiser and Norbert Esser — Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V, Department Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany

Laser spectroscopic methods for investigations of surface optical properties often require high incident excitation power (in MW/cm^2 range) leading to considerable heating effects which distort the measurements results. In many cases the heat transfer from the surface is hindered by interface effects or unfavorable substrate characteristics (e.g. low heat

conductivity). A precise sample temperature determination becomes an issue, since conventional methods are not able to deliver a local temperature within the laser spot. An evaluation of Stokes to anti-Stokes ratios in Raman spectroscopy is a well-established in-situ method for local temperature measurements. However its imitation regarding a low signal to noise ratio and necessity for instrument corrections makes it often unfeasible. We propose a new vibrational spectroscopy based method for in-situ temperature determination on surfaces minimizing these drawbacks by exploiting the low energy Stokes and anti- Stokes range in Raman spectra. As an example temperature measurements on (4×1) metallic In nanowires on Si(111) in the range between 50 K and 450 K will be shown.