HL 42: Oxide semiconductors

Time: Wednesday 9:30–12:15 Location: POT 51

HL 42.1 Wed 9:30 POT 51

Modelling native defects in transparent conducting oxides using the hybrid QM/MM embedded cluster technique — •Qing Hou, John Buckeridge, Alexey A. Sokol, Jingcheng Guan, and C. Richard A. Catlow — Kathleen Lonsdale Materials Chemistry, Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, UK

For n-type transparent conducting oxide (TCO) materials such as SnO2, In2O3 and ZnO, native defects play a key role in electronic conductivity. Depending on their electronic structure, energetics and geometries, defects can act as donors, resulting in intrinsic n-type conductivity, or can compensate extrinsic donors such as Sn in In2O3. Predictive modelling of the properties of defects in such systems requires a detailed description of the dielectric response of the host material, which can be difficult to obtain using standard supercell techniques. Here, we employ the hybrid quantum mechanical/molecular mechanical (QM/MM) embedded cluster method, a multi-region approach that allows us to model defects at the true dilute limit, with polarisation effects described in an accurate and consistent manner. Moreover, we develop techniques to analyse the energetic balance between electrons bound to donors in diffuse and compact states, a difficult problem regardless of the model employed. We benchmark our results where possible and find good agreement with experiments for a variety of defect-related properties.

HL 42.2 Wed 9:45 POT 51

CVD based growth of ZnO layers on Si(111) w/ and w/o AlN nucleation layers. — •Raphael Müller[1], Okan Gelme[1], Florian Huber[1], Jan-Patrick Scholz[2], Martin Mangold[1], Alexander Minkow[2], Ulrich Herr[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University — [2]Institute for Functional Nanosystems, Ulm University

The epitaxial growth of high quality zinc oxide (ZnO) layers on silicon (Si(111)) is a challenging task, because the formation of an amorphous SiO_x layer at the interface usually inhibits the growth of a well oriented ZnO layer. One way to circumvent this is the prior growth of a thin AlN nucleation layer, grown by MOVPE. Such nucleation layers were optimized and finally overgrown with ZnO layers under different growth conditions by a chemical vapor deposition (CVD)-based growth method, in order to find the best combination of growth parameters for both processes. The resulting ZnO layer quality was characterized by atomic force microscopy, electron backscattering diffraction, high resolution X-ray diffraction, low temperature photoluminescence and high resolution TEM measurements. A drastic increase in layer quality was observed comparing such layers to those w/o AlN nucleation layer, proofing the critical role of SiO_x at the interface. Growth temperature and thickness of the AlN nucleation are critical parameters, too, and have to be adjusted, as well as the temperature and II/VI-ratio of the ZnO growth. Finally we achieved perfectly aligned ZnO layers with a surface roughness RMS value of $1.2\,nm$, and a FWHM in ω-scan of $715\,arcsec$ for the ZnO (0002) reflection.

HL 42.3 Wed 10:00 POT 51

Magnetic-field-induced second harmonic generation of excitons in Cu_2O — •Andreas Farenbruch, Johannes Mund, Dietmar Fröhlich, Dmitri Yakovlev, and Manfred Bayer — Experimentelle Physik 2, Technische Universität Dortmund, Germany

We report on magnetic-field-induced second harmonic generation (SHG) of higher excitons ($n \geq 3$) of the lowest exciton series in Cu_2O. SHG is allowed for the $1S$ orthoexciton and higher excitons in low symmetry directions (e.g. [111] and [112]). By application of a magnetic field in Voigt geometry SHG gets also allowed for excitation along the [110]-axis. Magnetic-field experiments in Voigt configuration are of special interest, since one expects besides the Zeeman effect also the magneto-Stark effect, which leads to an effective electric field perpendicular to the light propagation and magnetic-field direction. With a group theoretical analysis we derive polarization selection rules for SHG. Of special elegance are 2D polarization diagrams (SHG intensity versus incoming and outgoing polarization angle). By a special choice of the experimental settings one can separate the spectral features due to the Zeeman effect and the magneto-Stark effect or observe an interference of both effects. The SHG signals are large enough to measure the full polarization dependence for the whole spectrum. It is shown, that the magneto-Stark effect dominates the Zeeman effect for higher principal quantum numbers.

HL 42.4 Wed 10:15 POT 51

A Koopman*s compliant exchange correlation potential for semiconductors — •Michael Lorke, Peter Deak, and Thomas Frauenheim — BCCMS, Universität Bremen

Density functional theory is the workhorse of theoretical materials investigations. Due to the shortcoming of (semi-)local exchange correlation potentials, hybrid functionals have been established for practical calculations to describe surfaces, molecular adsorption, and defects. These functionals operate by mixing between semi-local and Hartree-Fock exchange semi-emprically. However, their parameters have to be optimized for every material separately. To treat materials with a more physics driven approach and without the need of parameter optimization is possible with many-body approaches like GW, but at an immense increase in computational costs and without the access to total energies and hence geometry optimization.

HL 42.5 Wed 10:30 POT 51

Investigations on the electronic structure of strongly correlated electron system Cr-doped PrFeO3 — •Anil Kumar. and Pankaj R Sagdeo — Indian Institute of technology Indore, Indore-453552, India

High-resolution powder x-ray diffraction (SXRD), Soft x-ray absorption (SXAS) Raman and optical absorption spectroscopy (OAS) studies have been carried out to estimate the possible correlation between tolerance factor, structural bandwidth (w) , eg electron bandwidth (W) estimated from SXAS and charge transfer parameter (Δ) on one of the strongly correlated system Cr-doped PrFeO3. The present investigation suggests that tolerance factor, w and W scale in a similar fashion with Cr-doping, which infers the governance of these parameters by a common factor. The observed variation in eg electron bandwidth and has been understood in terms of variation in the Fe-O bond length and Fe-O-Fe bond angles with Cr-doping, which enhances the overlapping between Fe-O orbitals. Further, Resonant and power dependent Raman spectroscopy experiments were carried out to understand the origin of local oxygen breathing mode in the mixed Fe-Cr orthorhombic perovskite through the orbital mediated electron-phonon coupling (EPC) mechanism. Thus, by using the combination of SXAS, SXRD, Raman and OAS, a crucial information related to tolerance factor, structural bandwidth, eg electron bandwidth and Δ has been demonstrated. Additionally, present investigations strongly reveal the orbital mediated EPC is not limited to Jahn-Teller active materials and this series can be used as a model for study on orbital mediated EPC.

30 min. break

HL 42.6 Wed 11:15 POT 51

Highly Doped Transparent Conductive Oxides — •Alexander Koch, Jura Rensberg, Martin Hafermann, and Carsten Ronning — Institute of Solid State Physics, Friedrich-Schiller University Jena

Transparent conductive oxides have recently gained a lot of attention for applications in plasmonics and nanophotonics due to their low optical loss, metal-like behavior, tailorable optical properties, and well-established fabrication procedures. In particular, n-type doped zinc oxide (ZnO), such as gallium doped ZnO (GZO) is very attractive, because its dielectric permittivity can be engineered over a broad range from near to far IR. Here we show, that a very high doping concentrations in GZO can be reached by ion implantation and post implantation annealing treatment, where we have to face the competition between dopant activation and dopant diffusion. Furthermore, ion implantation offers the great opportunity to selectively dope ZnO by using appropriate lithography techniques. By this means, subwavelength structure elements, typically used for metasurfaces, fabrication can be formed.

HL 42.7 Wed 11:30 POT 51

Exciton Lattices in Curprous Oxide — •Martin Bergen — Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany

Excitons are a heavily studied topic within the field of semiconductor physics and generally well understood. For example they can be created in highly excited states as so called Rydberg-excitons. This specific form of exciton is characterized by a large spatial extension and strong interaction between the excitons as well as external fields. However, currently only a few select materials with comparatively large binding energies like cuprous oxide (Cu_2O) can be effectively studied. In Cu_2O excited states with principal quantum number up to n=25 can be observed, which corresponds to an exciton extension of over $2\,\mu m$. Due to the large dipole-dipole interaction a so called Rydberg-blockade can be observed, which prevents the creation of additional excitons in the vicinity of already existing excitons.
In atom physics optical lattices with cold atoms are an often used tool to study the atom's physics. In analogy to this our most recent findings on the influence of lattices on Rydberg-excitons in Cu_2O will be shown. One example is an enhanced Rydberg-blockade as compared to a homogeneous exciton distributon.

HL 42.8 Wed 11:45 POT 51

H_2S detection for medical breath analysis with surface functionalized ZnO nanowires — •Angelika Kaiser[1], Erick Torres[1], Tanja Mauritz[1], Yujia Liu[1], Florian Huber[1], Ulrich Herr[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter, Ulm University — [2]Institute of Functional Nanosystems, Ulm University

Numerous publications in the past years highlighted the potential importance of hydrogen sulfide (H_2S) detection for therapeutic applications and early diagnostics. It was suggested that an abnormal production of H_2S in the human respiratory system functions as an early biomarker for inflammatory diseases like asthma etc. Reliable breath analysis with respect to H_2S detection demands a reproducible and selective sensor device. Therefore, we present a planar resistive gas sensor based on the gas sensing approach of a ChemFET for medical breath analysis in an electronic nose approach. Here, the CVD grown zinc oxide (ZnO) nanowire (NW) surface operates as the gas sensitive open gate, while the conductive core serves as the source-drain channel. We investigated the benefit of surface modification of ZnO NWs, which are used for the detection of gaseous H_2S in the very low parts per billion (ppb) concentration range. In particular, we studied the catalytic effect of thin nanoparticle layers of gold (Au) or platinum (Pt) deposited on the ZnO NW surface in order to improve H_2S sensor sensitivity, selectivity and limit of detection. We find that surface modification with Au nanoparticles improves the overall sensor performance and allows for an exceptional detection limit below 10 ppb for H_2S diluted in synthetic air at room temperature.

HL 42.9 Wed 12:00 POT 51

defect compensation in the p-type transparent oxide Ba2BiTaO6 — •Diana Dahliah, Gian-Marco Rignanese, and Geoffroy Hautier — institute of Condensed Matter and Nanoscience (IMCN), Universit e catholique de Louvain (UCLouvain), Louvain-la-Neuve, Belgium

Transparent Conducting Oxides TCOs, combine a wide bandgap with good conductivity properties, such an unusual combination can be obtained by doping (n-type or p-type) a wide band gap oxide. p-type conductors are lagging behind in their performance because of the low hole mobility due to the presence of localized O 2p orbitals in the valence band. Breaking this localization and finding a p-type material with good conductivity as the one of n-type TCOs will make a revolution in the industry and will flip the type of materials that are used in some industrial applications. In a recent paper, Ba2BiTaO6 was reported as remarkable high mobility p-type TCOs though its conductivity is limited by charge compensation[1]. Here, we used first principles computations to investigate the reasons behind such a low conductivity from a defects physics standpoint. The calculated defect formation energies confirm that K is an adequate p-type shallow extrinsic dopant but that high p-type doping is prevented by the presence of compensating defects. Our work stresses the inherent difficulty in doping Ba2BiTaO6, we also highlight the potential directions for future improvements in its conductivity.

[1] A. Bhatia et al., Chem. Mater. 28, 30-34 (2016)