DS 48: Oxide Semiconductors (jointly with HL)

Time: Friday 9:30–12:45 Location: POT 51

Invited Talk DS 48.1 Fri 9:30 POT 51

New Frontiers in Quantum Matter Heterostructures — •Jochen Mannhart — Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Combining the power and possibilities of heterostructure engineering with the collective and emergent properties of quantum materials, quantum-matter heterostructures [1] open a new arena of solid-state physics. Here we provide a review of interfaces and heterostructures made of quantum matter. As we will show, unique electronic states can be engineered in these structures, giving rise to unforeseeable opportunities for scientific discovery and potential applications.

[1] Quantum-Matter Heterostructures, H. Boschker and J. Mannhart, Annual Reviews of Condensed Matter Physics, 8, April 2017.

DS 48.2 Fri 10:00 POT 51

Self-consistent hybrid functional calculations: Electronic and optical properties of oxide semiconductors — •Daniel Fritsch[1], Benjamin Morgan[1], and Aron Walsh[1,2] — [1]Department of Chemistry, University of Bath, BA2 7AY Bath, UK — [2]Department of Materials, Imperial College London, SW7 2AZ London, UK

Owing to limitations of existing approximate exchange-correlation functionals, band gaps of semiconductors and insulators are often severely underestimated in density functional theory calculations. Considerable improvements are possible by including a fraction of Hartree-Fock exchange, constructing a so-called "hybrid" functional. The precise proportion of Hartree-Fock exchange is typically treated as an empirical parameter chosen from intuition and experimental calibration.

A recent self-consistent hybrid functional [1] removes this empiricism and offers a new approach for parameter-free hybrid functional investigations. Moreover, it provides a better starting point for many-body perturbation calculations based on the *GW* approximation. Applying this approach to a range of oxide semiconductors, we report on the electronic and optical properties, and compare them to other theoretical and experimental data.

[1] J. H. Skone *et al.*, Phys. Rev. B **89**, 195112 (2014).

DS 48.3 Fri 10:15 POT 51

Influence of temperature on the creation of Rydberg excitons — •Peter Grünwald[1], Julian Heckötter[2], Marc Assmann[2], Dietmar Fröhlich[2], Manfred Bayer[2], Heinrich Stolz[1], and Stefan Scheel[1] — [1]Institut für Physik, Universität Rostock, Rostock, Germany — [2]Experimentelle Physik 2, TU Dortmund, Dortmund, Germany

Solid-state systems are heavily influenced by temperature, changing the crystal structure and thus shifting the energy bands [1,2]. Excitons in semiconductors additionally experience collision ionization, and a decrease of the band edge due to plasma interaction [3]. However, in most semiconductor systems, measuring these effects is difficult because of the limited number of exciton states available. This is different for Rydberg excitons [4], where states up to $n \gtrapprox 20$ can easily be generated. Hence, these states can be used to analyze the temperature influence on the excited states and the excitation limit set by finite temperature.

[1] T. Itoh and S. Narita, J. Phys. Soc. Japan **39**, 140 (1975).
[2] P. B. Allen and M. Cardona, Phys. Rev. B **23**, 1495 (1980).
[3] D. Semkat *et al.*, Phys. Rev. B **80**, 155201 (2009).
[4] T. Kazimierczuk *et al.*, Nature **514**, 343 (2014).

DS 48.4 Fri 10:30 POT 51

Excitonic Giant-Dipole Potentials in Cuprous Oxide — •Markus Kurz and Stefan Scheel — AG Quantenoptik makroskopischer Systeme, Institut für Physik, Universität Rostock

Wannier excitons are of great physical interest since they represent the fundamental optical excitation in semiconductors. Recently, the discovery of highly excited Rydberg excitons in Cuprous Oxide (Cu_2O) and their exposure to external fields have shown a plethora of complex physical phenomena [1]. In atomic physics an exotic species of Rydberg atoms in crossed electric and magnetic fields, so-called giant-dipole atoms, have been predicted for two decades [2]. These exotic objects are characterized by an electron-ionic core separation in the range of several micrometers.

In this work, we expand this concept and predict the existence of excitonic giant-dipole states in Cu_2O. Performing a gauge-independent pseudoseparation of the center of mass motion we derive an effective single-particle description of the field-dressed excitonic system obtaining a spatial dependent electron-hole interaction potential. For specific field strengths and field orientations this potential exhibits an outer potential well providing bound excitonic states. Furthermore, we show that the giant-dipole interaction potential gives rise to Abelian and non-Abelian gauge fields acting on the relative motion of the two excitonic constituents.

[1]T. Kazimierczuk *et al.*, Nature (London) **514**, 343 (2014)
[2]O. Dippel, *et al.*, Phys. Rev. A **49**, 4415 (1994)

DS 48.5 Fri 10:45 POT 51

Excitons at $SrTiO_3$ and ZnO interfaces in ellipsometry spectra — •Stefan Zollner[1], C. Rodriguez[1], N. Samarasingha[1], J. Moya[1], N. Fernando[1], P. Ponath[2], K. Kormondy[2], A.A. Demkov[2], and S. Chattopadhyay[3] — [1]New Mexico State University, Las Cruces, NM, USA — [2]University of Texas, Austin, TX, USA — [3]Indian Institute of Technology, Indore, India

Excitonic features in optical spectra of semiconductors and insulators have been studied for many years. In an epitaxial layer on a substrate with a different band gap, the wave functions of electron and hole are strongly modified. In a type-I quantum well, consisting of a narrow-gap semiconductor grown on a large-gap substrate, both electron and hole are confined, which leads to an increase in the dipole overlap matrix element. Therefore, the dominant absorption peak at 4.2 eV is larger in a 20 nm thick $SrTiO_3$ layer on $LaAlO_3$ than in bulk $SrTiO_3$. (The band gap of $LaAlO_3$ is larger than that of $SrTiO_3$.) On the other hand, in a staggered type-II quantum well, either the electron is confined, or the hole, but not both. Therefore, the overlap dipole matrix element (and the excitonic absorption) is strongly reduced, because one quasiparticle resides in the quantum well and the other in the substrate. If a $SrTiO_3$ layer is grown on Si or Ge, the valence band maximum occurs in the substrate, while the conduction band offset is very small. Therefore, the exciton wave function is delocalized, which reduces the dipole overlap matrix element. The real and imaginary part of thin SrTiO3 layers on Si or Ge are much smaller than in the bulk and decrease monotonically with decreasing thickness.

Coffee Break

DS 48.6 Fri 11:30 POT 51

Tuning the refractive index of transparent conducting oxides via oxide/oxide periodic heterostructures — David Caffrey, Emma Norton, Cormac Ó Coileáin, Christopher M. Smith, Igor V. Shvets, and •Karsten Fleischer — School of Physics and CRANN, Trinity College Dublin, The University of Dublin, Ireland

Superlattice structures are a novel method of improving upon the optoelectronic properties of Transparent Conducting Oxide (TCO) structures. The invariability of the refractive index of TCO materials leads to reflection losses cells. The development of a transparent material or structure of tuneable refractive index at the interfaces of transparent devices such as solar would allow for the integration of anti-reflective coatings which would reduce such losses significantly, thus improving device efficiency. Previous attempts to modify the refractive index have been marred by the degradation of the electrical or optical properties of the tuned material. We demonstrate the novel use of a TCO/dielectric superlattice structure to achieve an effective medium of altered refractive index, while maintaining high values of transparency, conductivity and mobility. We demonstrate the efficacy of these superlattice structures on both amorphous $InGaZnO_4$ and ZnO:Al via TCO/SiO_2 and TCO/TiO_2 superlattices. The effective refractive indices of the films were successfully tuned over a range of $\Delta n \approx -0.2$ (SiO_2 inclusion) to $+0.4$ (TiO_2 inclusion) with a decrease in conductivity of less than an order of magnitude. Mobility of the films was also well conserved. We also discuss differences in the carrier injection from the TCO into the dielectric for the SiO_2 and TiO_2 case.

DS 48.7 Fri 11:45 POT 51

Hybrid functional calculations of oxygen mono- and di- vacancies in SrTiO3 — •Masud Alam, Liverios Lymperakis, and Jörg Neugebauer — Computational Material Design department, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck Str. 1, 40237 Düsseldorf, Germany

Perovskite-type oxides ABO3 have attracted considerable interest for their large variety of technologically appealing characteristics such as ferroelectricity, magnetism, as well their dielectric properties. Among these materials, SrTiO3 (STO) serves as a representative model for the class of large bandgap perovskites. Nevertheless, the properties of this material are dominated by the presence of oxygen vacancies which act as n-type dopants. In the present work we investigate the energetics, atomic geometry and electronic structures of oxygen mono- and di-vacancies by employing Heyd, Scuseria, Ernzerhof (HSE) hybrid density functional calculations. Based on these calculations we identify the energy levels and the formation energies of aforementioned point defects as well as the binding energies of the point defect complexes. Our calculations reveal that interactions between single and doubly ionized defects as expected are strongly repulsive. Based on the aforementioned results we will further discuss in details the effect of oxygen vacancies as a function of growth conditions and doping level on the electronic properties of STO.

DS 48.8 Fri 12:00 POT 51

Low temperature absorption study of ferromagnetic EuO thin films — •Marcel Ney[1], Günther Prinz[1], Timm Gerber[2], Martina Müller[1,2], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, Universität Duisburg-Essen, D-47048 Duisburg — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, D-52428 Jülich

Europium Oxide is a ferromagnetic semiconductor with the Curie temperature of 69K. When it is used as a tunnel barrier, it can create up to 100% spin polarized electron currents, for use in spintronic research. This remarkable property raises the question, how the magnetic order at low temperatures affects the band structure of a thin EuO layer.

Thin EuO-layers were grown by molecular beam epitaxy on yttria-stabilized-zirconia-substrates, with different thicknesses. A fourier-transform-infrared spectrometer equipped with a liquid helium continuous-flow cryostat was used to measure the transmission through the EuO thin films.

Spectra measured for decreasing EuO thickness (30nm-3nm) show a shift of the absorption edge of EuO to higher energies due to an increasing quantum confinement along the growth direction. For low temperature measurements below the Curie temperature of EuO, we observed a red shift of the bandgap energy of about $E_a = (0.27 \pm 0.02)$eV. This energy shift is in good agreement with theoretical values and experimentally determined exchange splitting energies for thin europium-oxide layers, already published in the literature.

DS 48.9 Fri 12:15 POT 51

Ozone, oxygen and water interaction with In_2O_3(111) surfaces — •Theresa Berthold[1], Stefan Krischok[1], Marcel Himmerlich[1], Vladimir Polyakov[2], Volker Cimalla[2], Julius Rombach[3], and Oliver Bierwagen[3] — [1]Institut für Mikro- und Nanotechnologien MacroNano, Technische Universität Ilmenau — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Freiburg — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin

In_2O_3 films are widely used in conductometric gas sensors based on their surface electron accumulation layer (SEAL) whose conductance is influenced by gas adsorption [1]. In this study the chemical composition and electronic surface properties of undoped and Mg-doped In_2O_3(111) films grown by plasma-assisted molecular beam epitaxy are analyzed by photoelectron spectroscopy. We analyze the formation or desorption (by UHV annealing or UV illumination) of adsorbates, the generation of defects as well as the variation in surface band bending, electron concentration, and surface dipole. Towards understanding the gas sensitivity under realistic conditions we study the effect of humidity on the sensor properties by experiments combining water interaction with ozone or oxygen surface oxidation. H_2O partially reverses the depletion/reduction of the SEAL after surface oxidation. Complete depletion of the SEAL is found after plasma oxidation [2]. The experimental results are combined with Schrödinger-Poisson calculations to establish a quantitative analysis of the electron density profile and the density of surface states. [1] J. Rombach et al., Sens. Actuators B, 236, 909 (2016) [2] T. Berthold et al., J. Appl. Phys. (submitted)

DS 48.10 Fri 12:30 POT 51

Gas sensing with sub-micrometer Pt/TiO_2 sensors — •Svenja Herbertz, Mihai Cerchez, and Thomas Heinzel — Solid State Physics Laboratory, Heinrich-Heine-Universität Düsseldorf

Pt/nanoporous TiO_2 hydrogen sensors with active sizes in the millimeter regime are technically well established although the underlying physics is still at debate, due to incomplete understanding of the interplay between oxygen vacancies, titanium interstitials, and hydrogen incorporation in this disordered system. The quest for miniaturization as well as for improved spatial resolution drives the search for sensors operational at the microscale. Here we present a sub-micrometer-sized lateral sensor for atmospheric hydrogen with planar geometry and full compatibility with Si processing technology. A titanium dioxide line of 200 nm width, written with the tip of an atomic force microscope, separates a thin Ti film on an insulating substrate into two metallically disconnected electrodes and forms the active area. It is sensitized by a sub-monolayer platinum sputtering step such that the two Ti electrodes remain disconnected. The device shows a large, selective sensitivity to hydrogen gas.