HL 38: Oxide Semiconductors II

Oxide Semiconductors except for ZnO

Time: Tuesday 14:45–15:45 Location: H13

HL 38.1 Tue 14:45 H13

Signatures of quantum coherence in Rydberg excitons in Cu_2O — •Peter Grünwald[1], Marc Assmann[2], Dietmar Fröhlich[2], Manfred Bayer[2], Heinrich Stolz[1], and Stefan Scheel[1] — [1]Institut für Physik, Universität Rostock, D-18059 Rostock, Germany — [2]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany

In a recent breakthrough experiment, excitons in Cu_2O have been optically excited to Rydberg states with principal quantum numbers upto $n = 25$ [1]. These fragile objects show very similar behaviour compared to their atomic counterpart, including the concept of a quantum defect [2].

We present first results on the study of the quantum optical properties of Rydberg excitons. The details of the absorption spectrum of excitons with large n can only be understood by including coherent excitation dynamics [3]. The measured absorption spectrum includes both the probability for absorbing a laser photon as well as a contribution relating to the coherent and incoherent parts of the intensity spectrum of the excitons. For increasing n, the incoherent spectrum becomes relevant. In particular, additional resonances appear between the exciton peaks, which vanish if the laser pumping is substituted for white-light excitation. These resonances indicate the onset of quantum-coherent light-exciton interaction.

[1] T. Kazimierczuk *et al.*, Nature **514**, 343 (2014).
[2] F. Schöne *et al.*, arXiv:1511.05458 [cond-mat.mes-hall].
[3] P. Grünwald *et al.*, arXiv:1511.07742 [cond-mat.mes-hall].

HL 38.2 Tue 15:00 H13

Hybrid density functional calculations of small polarons and bi-polarons in oxides — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz Haber Institute of the MPS, Berlin, Germany

Formation of polarons, i.e. phonon-"dressed" holes or electrons, plays an important role in optical spectra and electrical conductivity of materials. For the formation of small (localized) polarons microscopic properties of the systems are crucial, and the use of an *ab initio* theory is necessary for its description. For this reason we calculate small polarons in a supercell approach using density functional approximations (DFA).

We find that the results can be strongly affected by self-interaction and finite supercell size errors. However, using constraints from exact DFT, such as the IP-theorem[1], the binding energy of polarons can be reformulated in terms of energies obtained from the neutral system[2]. With this we show, that the dependence on the underlying XC functional of the reformulated polaron binding energy can be drastically reduced. The effect will be demonstrated for small polarons and bi-polarons in MgO for the entire range of the the exact-exchange fraction in the HSE hybrid functional. We also demonstrate the dependence of the results on the supercell size and give results on the binding energies of polarons in the extrapolated dilute limit.

[1] J. Perdew et al., Phys. Rev. Lett. **49**, 1691 (1982) [2] B. Sadigh Phys. Rev. B **92**, 075202 (2015)

HL 38.3 Tue 15:15 H13

Stark-Effect Measurements on Rydberg Excitons in Cu_2O — •Marcel Freitag, Julian Heckötter, Marc Assmann, Dietmar Fröhlich, and Manfred Bayer — Technische Universität Dortmund, Fakultät Physik, Experimentelle Physik II, 44221 Dortmund, Germany

We report on Stark-Effect measurements of Rydberg excitons[1] in Cu_2O with quantum numbers up to $n = 25$. These excitons have extensions up to $2\,\mu$m. As known from hydrogen, the dipole matrix elements for $\Delta n = 0$ and $\Delta l = \pm 1$ grow quadratically with n. Due to the electric field induced coupling, we observe S- and D-excitons of the yellow series and from $n = 5$ we are even able to identify G-excitons in fields as low as $50\,\mathrm{V/cm}$. Measurements are done on a $30\,\mu$m sample with a single frequency dye laser ($\Delta E = 5$ neV) and a broadband white-light source at temperatures down to 1.2 K. Contrary to hydrogen, the Stark-Effect measurements can be done in a longitudinal configuration ($K_{laser} \parallel E$).

[1] T. Kazimierzuk et al. Nature 514, 343 (2014)

HL 38.4 Tue 15:30 H13

Optical properties of β -Ga_2O_3 — •Nadja Jankowski[1], Christian Nenstiel[1], Gordon Callsen[1], Zbigniew Galazka[2], and Axel Hoffmann[1] — [1]Technische Universität Berlin, Berlin, Deutschland — [2]Leibniz Institut für Kristallzüchtung, Berlin, Deutschland

β-Ga_2O_3 is a wide band gap semiconductor, which is suitable for many possible applications, such as transparent conducting oxides, UV-devices, high-temperature-stable gas sensors and dielectric coating for solar cells.

Structural and optical properties of the investigated β-Ga_2O_3 single crystal were examined by the means of Raman and photoluminescence spectroscopy.

As the exact band gap value of β-Ga_2O_3 is still under discussion, this work focuses on the determination of the band gap by performing photoluminescence excitation spectroscopy. The measurements exhibit excitation channels in the region of 4.6 to 5.0 eV, below the theoretically calculated band gap within recent publications. To clarify the origin of the excitation channel at 4.91 eV, temperature dependent photoluminescence excitation spectroscopy and absorption spectroscopy were performed.