HL 58: Focus Session: Copper oxide semiconductors – An attractive material for photovoltaics?

The p-type conducting copper-oxide compound semiconductors (Cu_2O, CuO) provide a unique possibility to tune the band gap energies from 2.1 eV to the infrared at 1.40 eV into the middle of the efficiency maximum for solar cell applications. By a pronounced non-stoichiometry the electronic properties may vary from insulating to metallic conduction. They appear to be an attractive alternative absorber material in terms of abundance, sustainability, non-toxicity of the elements, and numerous methods for thin film deposition that facilitate low cost production. The future and possible limitations of copper-oxide based thin-film solar-cells will be discussed by a critical look at their established physical properties and at those which need to be further investigated and improved (Organizers: Christian Heiliger, JLU Gießen, and Carsten Ronning, FSU Jena).

Time: Wednesday 15:00–18:00 Location: H13

Topical Talk HL 58.1 Wed 15:00 H13

Potential and possibilities of copper oxide compounds — •Bruno K. Meyer — 1. Physics Institute, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Many current thin film materials used in photovoltaics have resource limitations e.g. $CdTe$, CIGS. Earth Abundant Semiconductors such as Cu_2O, Zn_3P_2, or FeS_2 are currently under investigations since apart from abundance, sustainability, non-toxicity of the elements, and numerous methods for thin film deposition that facilitate low cost production are equally important aspects. In the talk the synthesis and characterisation of Cu_2O thin films used as p-type absorbers in heterojunction solar cells will be reported. We discuss i) controlled p-type doping by nitrogen ii) the role of the possible n-type dopant Zn, and iii) tuning of the energy gap by alloy formation.

Topical Talk HL 58.2 Wed 15:30 H13

Intrinsic and hydrogen related impurities in Cu_2O — •Graeme Watson — School of Chemistry and CRANN, Trinity College Dublin, Dublin 2, Ireland

Cuprous oxide (Cu_2O) is a prototypical p-type conducting oxide with applications in dilute magnetic semiconductors, low cost solar cells, gas sensors and catalysis. It is also the parent compound of many p-type transparent conducting oxides (TCOs), which are thought to retain the valence band features and conduction mechanisms of Cu_2O. Understanding conduction in Cu_2O is therefore vital to the optimization of Cu-based materials for many applications. Calculation of the native defects in Cu_2O show that GGA and GGA+U are not capable of obtaining an accurate description of the polaronic nature of p-type defects in Cu_2O,[1] however, hybrid-DFT yields deep single-particle levels, consistent with experimentally observed activated, polaronic conduction. Our calculated transition levels for simple and split copper vacancies explain for the first time the source of the two distinct hole states seen in DLTS experiments [2] and demonstrate that Cu_2O can never be made n-type by native defects.[3] We also investigate the behaviour of hydrogen in Cu_2O,[4] and elucidate the "quasi-atomic" hydrogen site that Muon spectroscopy has been unable to identify. We discuss the impact of H on the electrical properties of Cu_2O-based materials, and propose methods to increase device performance.

[1] J. Chem. Phys., 131, 124703 (2009), [2] Phys. Rev. Lett., 103, 096405 (2009), [3] J. Phys. Chem. Lett. 1, 2582 (2010), [4] Phys. Rev. Lett., 106, 186403 (2011)

HL 58.3 Wed 16:00 H13

Molecular Beam Epitaxy of copper oxides (mainly cuprous oxide Cu_2O) — •Max Kracht, Jörg Schörmann, Thomas Sander, Peter J. Klar, and Martin Eickhoff — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

Semiconducting binary oxides (SBOs) are currently gaining intense research interest. Within this class of materials the copper oxide system (Cu-O) with the two stable phases cubic Cu_2O (cuprous oxide) and monoclinic CuO (cupric oxide) presents a fascinating exception both in terms of its electronic and its optical properties. The different Cu-O phases possess optical band gaps in the visible part of the spectrum ($E_g(Cu_2O) = 2.1\ eV$, $E_g(CuO) = 1.4\ eV$ at RT) which makes them suitable for application as absorber layers in photovoltaic devices. Cu-O thin films were grown by plasma assisted molecular beam epitaxy (PAMBE) on MgO substrates. An increase of flux ratio of Cu/O leads to a phase transition from CuO to Cu_2O which means that the phase can be controlled by the adjustment of stochiometrie of the deposited layer. Phase pure Cu_2O films were achieved at a substrate temperature of 700 $°C$, as demonstrated by high resolution x-ray diffraction and Raman spectroscopy. For the growth of $Cu_2O(001)$ on $MgO(001)$ substrates the appearance of (011) misorientations, i.e. the growth rate on the different facets, has been found to be sensitively controllable and supressed by the Cu/O ratio during PAMBE growth. Hall-Effect measurements reveal a p-type carrier concentration of $6.1 \cdot 10^{15}\ cm^{-3}$ and a mobility of 47.2 $\frac{cm^2}{Vs}$ for Cu_2O films.

Coffee break

Topical Talk HL 58.4 Wed 16:45 H13

Accelerating efficiency enhancements in cuprous oxide thin films by applying a structured approach — •Tonio Buonassisi — Massachusetts Institute of Technology, Cambridge, MA 02139, USA

With the exception of cuprous sulfide (Cu2S), binary Earth-abundant photovoltaic compounds (FeS2, Cu2O, SnS...) have record conversion efficiencies of a few percent or less, despite decades of research. It has recently been questioned whether these materials are intrinsically limited, or whether further efficiency improvements are possible with a structured scientific approach. In this presentation, we will present evidence supporting the latter hypothesis, demonstrating how a systematic approach to absorber and buffer layer development can accelerate efficiency improvements in certain Earth-abundant compounds. This systematic approach, mirroring the successes of more traditional semiconductor compounds, features multiscale modeling and interface engineering as cornerstones of a concerted effort to improve device performance. We postulate that this systematic approach to improving device performance may extend to a wider range of Earth-abundant absorber materials, potentially increasing the range of "serious" candidate solar cell materials at a historically high rate.

Topical Talk HL 58.5 Wed 17:15 H13

Photoemission Spectra of CuO from First Principles: Quasiparticle Excitations and Beyond — •Claudia Rödl, Francesco Sottile, and Lucia Reining — Laboratoire des Solides Irradiés, Ecole Polytechnique, CEA-DSM, CNRS, 91128 Palaiseau cedex, France and European Theoretical Spectroscopy Facility (ETSF)

The insulating transition-metal oxide CuO constitutes the crucial building block of the high-temperature superconducting cuprates. The almost square-planar coordination of Cu with O together with an electron-correlation-induced coupling of the Cu 3*d* orbitals is assumed to be responsible for high-temperature superconductivity. In order to shed light on the electron-correlation effects in CuO, we aim for the full *ab initio* description of its photoemission spectrum capturing both quasiparticle and satellite excitations. Photoemission satellites are due to a coupling of the one-particle excitations to other excitations in the system (e.g. plasmons) and, hence, a sign of correlation.

We calculate the photoemission spectrum of CuO in the *GW* approximation (GWA) of many-body perturbation theory. Besides studying quasiparticle excitations and their life times, we focus on satellite structures. The energy loss that is due to plasmon excitations is obtained from time-dependent density-functional theory (TDDFT). Further, we will explore a recently developed approach to plasmon satellites that is based on an electron-boson coupling model and has already been applied successfully to simple *sp* semiconductors.

HL 58.6 Wed 17:45 H13

Band Structure and Optical Properties of Copper Oxide Compounds from First Principles — •Markus Heinemann and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-

Universität Gießen, Germany

Prospective applications in the fields of optoelectronics and solar technology raise the interest in the p-type semiconductors cuprous oxide (Cu2O), cupric oxide (CuO), and paramelaconite (Cu4O3) and demand a profound knowledge of the electronic and optical properties of these materials. While the electronic and optical properties of Cu2O are well investigated theoretically, there are only a few studies on the remaining two compouds where traditional methods within density functional theory (DFT) fail to describe the semiconducting state [1]. We present the results of our first principles DFT calculations of the band structure for all three compounds using ab initio methods beyond the LDA. We compare the DFT+U approach to hybrid functionals and quasiparticle calculations within the framework of the GW approximation. Further we assess the optical properties of the three copper oxide phases by calculating the dielectric function.

[1] B. K. Meyer, A. Polity, D. Reppin, M. Becker, P. Hering, P. J. Klar, Th. Sander, C. Reindl, J. Benz, M. Eickhoff, C. Heiliger, M. Heinemann, J. Blasing, A. Krost, S. Shokovets, C. Müller, and C. Ronning, Phys. Status Solidi B, 249: 1487-1509 (2012)