

HL 95: Novel Functional Materials II

Time: Friday 9:30–12:00

Location: H10

HL 95.1 Fri 9:30 H10

Electron traps in disordered Pt/TiO₂ hydrogen sensors — LAURIN SCHNORR¹, MIHAI CERCHEZ¹, DIETER OSTERMANN², and THOMAS HEINZEL¹ — ¹Heinrich Heine University Düsseldorf, Universitätsstr. 1D-40225 Düsseldorf — ²ODB-Tec GmbH & Co. KG, Bussardweg 12, 41468 Neuss, Germany

Hydrogen sensing at disordered Pt/TiO₂ interfaces lacks a deep understanding of the physical processes involved. Aspects related to the mechanism of electron conduction in such systems are attributed usually to oxygen vacancies and/or titanium interstitials. From an electronic transport point of view, defects manifest through creation of electronic states in the band gap, position of which is still under debate. Little is known about the effect of hydrogen on the band gap states during the sensing process. This knowledge would bring some more light concerning the physical hydrogen sensing mechanism. Here we make a step in this direction by performing deep level transient spectroscopy experiments [1] before, during, and after exposure to low concentrations of hydrogen. Our findings [2] suggest that two broad trap levels are present before the exposure, while a third level is formed during hydrogen exposure.

[1] D. V. Lang, *J. Appl. Phys.* 45, 3023 (1974). [2] L. Schnorr, M. Cerchez, D. Ostermann, and T. Heinzl, *Phys. Status Solidi B* (2015) (in press)

HL 95.2 Fri 9:45 H10

Theoretical and experimental study of the optoelectronic properties of Nb₃O₇(OH) and Nb₂O₅ for photochemistry — WILAYAT KHAN¹, SOPHIA B. BETZLER², ONDREJ SIPR¹, JIM CISTON³, PETER BLAHA⁴, CHRISTINA SCHEU⁵, and JAN MINAR^{1,2} — ¹Technologies-Research Center, University of West Bohemia, Univerzity 8, 306 14 Plzen, Czech Republic. — ²Department of chemistry and Center for NanoScience, Butenandtstrae 11, 81377 Munchen, Germany — ³National Center for Electron Microscopy, Lawrence Berkeley National Lab, Berkeley, USA. — ⁴Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria. — ⁵Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strae 1, Dusseldorf, Germany.

Nb₃O₇(OH) and Nb₂O₅ were proposed as high performing electrode materials in several fields of application such as dye-sensitized solar cells and photoelectrochemical cells. In this work, we present theoretical and experimental studies of Nb₃O₇(OH) and Nb₂O₅ to elucidate their optical and electronic properties. The theoretical study was performed using the full potential linearized augmented plane wave method to calculate the electronic band structures, the density of states and optical properties. To verify the results of our calculations energy-loss functions for the low-loss spectral region were calculated and compared to experimental electron energy-loss spectra, featuring a very close agreement between experiment and theory. Our investigations show that Nb₃O₇(OH) has more suitable optoelectronic and transport properties for photochemical application than Nb₂O₅.

HL 95.3 Fri 10:00 H10

Vibrational Properties of Thermoelectric Magnesium Silicides from First Principle: the role of explicit dopants — HAGEN - HENRIK KOWALSKI, LUCA GHIRINGHELLI, CHRISTIAN CARBOGNO, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Silicides, and particularly Mg₂Si, are simple, prototypical examples for thermoelectric materials and have thus recently attracted remarkable scientific interest. For this material class, most first-principles studies have so far focused on the structural stability, the electronic structure, and the electronic transport coefficients [1,2], viz. on how these properties can be tailored by doping. Little is however known about the effects of doping on the vibrational properties and the associated thermal conductivity, which are of similar importance for the thermoelectric efficiency. Therefore, we have systematically investigated how different dopants (Ca, Ge, Ag, etc.) affect the vibrational harmonic properties; anharmonic effects are analyzed within the quasi-harmonic approximation. We discuss the implications of our findings for the thermoelectric properties and how they can be utilized in a high-throughput framework.

[1] I. Opahle, G. K. H. Madsen, and R. Drautz, *PCCP* 14, 16197

(2012).

[2] S. Bhattacharya and G. K. H. Madsen, *Phys. Rev. B* 92, 085205 (2015).

30 min. Coffee Break

Invited Talk

HL 95.4 Fri 10:45 H10

Nano-architectures and organic-inorganic hybrid material combinations for novel photovoltaic device concepts — SILKE CHRISTIANSEN — Helmholtz-Zentrum- Berlin — Max-Planck-Institute for the Science of Light, Erlangen

The implementation of tailored nano-architectures into conventional inorganic and hybrid photovoltaic devices can improve photovoltaic (PV) cells by optimizing charge generation, separation and extraction. The charge generation can be improved through lowly reflective materials such as nano-patterned layers of silicon nanowires (SiNWs) or inverted cones (SiNCs), produced by reactive ion etching combined with nanosphere-lithography. Nanostructures with optimized optical behavior show large surfaces which require proper passivation e.g. by atomic layer deposition (ALD) and more importantly, good charge extraction concepts. These charge extraction concepts seek for novel cheap, transparent and highly conductive materials replacing conventional metal grid-electrodes. Interesting alternatives are solution-processed Ag-nanowire networks, stabilized and protected by e.g. ALD deposited aluminum doped ZnO, showing solar cells with high short circuit currents, low resistivity and small amounts of metal. The present paper shows optical behavior of individual and arrays of SiNWs and SiNCs in finite difference time domain (FDTD) simulations and experiments so that design rules for optimized PV cells can be derived. Experimental confirmation of simulations rely on nano-probing of individual nano-structures and ensembles using a powerful electron-microscopy platform capable of correlative microscopy and spectroscopies.

HL 95.5 Fri 11:15 H10

Electronic properties of freestanding Ti₃C₂T_x MXene monolayers — ALESSIO MIRANDA¹, JOSEPH HALIM², MICHEL W. BARSOUM², and AXEL LORKE¹ — ¹Dep. of Physics, Uni. Duisburg-Essen, Duisburg, 47058, Germany — ²Dep. of Materials Science and Engineering, Drexel University, Philadelphia, PA19104, USA

Recently, MXenes, 2D early transition metal carbides and carbonitrides, have been produced by the selective etching of A from the MAX phases. The latter are a large family of compounds, with the general formula M_{n+1}AX_n (n = 1-3), where M is an early transition metal, A is an A-group element, and X represents C or N [1]. During the etching process, the MXene surface acquires terminating functional groups, T, (namely -O, -OH, and/or -F), which can have significant effects on the work function and electrical properties of these new compounds. Here we report, on the electrical properties of Ti₃C₂T_x freestanding MXene monolayers in the 2.5 K to 300 K temperature range [2]. We show that Ti₃C₂T_x samples exhibit metallic behavior, they have a carrier density of 5 × 10¹⁴ cm⁻², which is relatively high and can be modulated by the application of a gate voltage. MXenes, which have already been demonstrated to be promising candidates for a variety of applications [3], may also be interesting for electronic applications, such as field-effect devices. Magnetotransport measurements are also reported.

[1] M. W. Barsoum, *MAX Phases: Properties of Machinable Ternary Carbides and Nitrides* (Wiley-VCH, 2013). [2] A. Miranda, et al. submitted (2015). [3] M. Naguib, et al *Adv. Mater.* 26, 992-1005 (2014).

HL 95.6 Fri 11:30 H10

Vibrational Dynamics of Filled Skutterudites — SUSMITA BASAK, CHRISTIAN CARBOGNO, and MATTHIAS SCHEFFLER — Fritz Haber Institute of the Max Planck Society

Skutterudites are promising candidates for thermoelectric applications, since their cage like structure can be filled with guest atoms to tune the electronic and vibrational properties and so to optimize the thermoelectric transport coefficients. Various conflicting phenomenological models (e.g., incoherent rattling, coherent coupling [1]) have been proposed to explain the interaction between guest and host, but the exact mechanisms are still topic of debate. To clarify this question, we determine the temperature dependence of the geometric, electronic, and

vibrational properties for a set of skutterudites (CoSb_3 , CoAs_3) and guests (Ga, In, Sn, etc.) using density-functional theory in the quasi-harmonic approximation. We find different coupling mechanisms to be active depending on the guest, which leads to a drastically different dynamics ranging from localized to coherent phonon modes. These modes, which are robust against doping and defy the common assumption that the guest's mass primarily determines the coupling, also largely influence the structural and electronic properties. Finally, we discuss the implications of our findings for controlling the thermoelectric efficiency. [1] M. M. Koza *et al.*, *Nat. Mat.* **7**, 805, (2008).

HL 95.7 Fri 11:45 H10

Formation and function of vacancies in Si/Ge Clathrates: The importance of broken symmetries — ●AMRITA BHATTACHARYA, CHRISTIAN CARBOGNO, and MATTHIAS SCHEFFLER — Fritz Haber Institute of the Max Planck Society

Inclusion compounds, such as clathrates, are cage-like crystal structures that can encapsulate guest atoms. Since this allows to granularly

tune their electronic and vibrational properties, they are regarded as interesting materials for thermoelectric applications. Progress in this field is, however, hindered by the fact that filling of group-IV clathrates often results in complex and unexpected structural changes, e.g., the spontaneous formation of vacancies in certain hosts: In Ge_{46} clathrates filled with K or Ba, the most favourable phases $\text{K}_8\text{Ge}_{44}/\text{Ba}_8\text{Ge}_{43}$ feature two/three vacancies. Conversely, the framework of the isoelectronic Si_{46} clathrate remains intact ($\text{K}_8\text{Si}_{46}/\text{Ba}_8\text{Si}_{46}$) upon filling with the exact same guests. Our first-principles calculations of the formation energies (including structural disorder as well as geometric and lattice relaxations) and of the thermodynamic phase stabilities (including harmonic free energies and configurational entropies) confirm this experimental scenario and shed light on the underlying mechanisms. Due to the spatially more delocalized $4sp^3$ orbitals in Ge, fundamentally different symmetry breaking distortions become possible to stabilize the vacancies compared to the more localized $3sp^3$ orbitals in Si. Eventually, we discuss the implications of these findings for the thermoelectric properties of clathrates.