HL 84: Novel Functional Materials I

Time: Thursday 14:45–17:30 Location: H17

Invited Talk HL 84.1 Thu 14:45 H17

Resonant plasmonic nanoantennas for mid-infrared spectroscopy and sensing — •Frank Neubrech and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University Stuttgart, Stuttgart

Plasmonic nanoantennas confine electromagnetic fields at infrared wavelengths to volumes of only a few cubic nanometers, resulting in huge local fields in the vicinity of the resonantly excited metal particles. These near fields are used to enhance the infrared vibrational bands of molecular monolayers and thus enable a spectroscopic detection with ultra-high sensitivity.[1,2] In the presentation, we will report on fundamental aspects of the vibrational enhancement in surface-enhanced infrared spectroscopy,[3,4] applications to infrared chemical imaging and sensing in life sciences, such as in-situ protein sensing. Additionally, we will present a combination of the above mentioned concept with a high power and broadband mid infrared laser source to further lower the detection limit in infrared spectroscopy.[5]

[1] F. Neubrech et al., Phys. Rev. Lett. **101**, 157403 (2008).
[2] D. Dregely et al., Nat. Commun. **4**, 2237 (2013).
[3] S. Bagheri et al., Adv. Opt. Mater. **11**, 1049 (2014).
[4] S. Bagheri et al., ACS Photonics **2**, 779 (2015).
[5] T. Steinle et al., Opt. Express **23**, 11105 (2015).

HL 84.2 Thu 15:15 H17

Tunable Coulomb-oscillations in improved CoPt nanoparticle based field-effect transistors — •Hauke Lehmann, Svenja Willing, Mirjam Volkmann, and Christian Klinke — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Metallic nanoparticles offer possibilities to build and improve basic electrical devices. The role of a semiconductor bandgap is adopted by the Coulomb energy gap due to the charging of the single particles capacities. Thus, it is required to keep the nanoparticles individualized by tunnel barriers, while a merging of the particles would render them metallic again.
We synthesize monodisperse CoPt nanoparticles by colloidal chemistry. Those particles are deposited via the Langmuir-Blodgett technique as highly-ordered homogeneous monolayers onto substrates with predefined gold electrodes. Additional structuring of the films yields stripes from individual nanoparticles. A local back-gate electrode is employed underneath the channel to influence the transport. This enables good electrostatic control over individually addressable devices without interferences from a dielectric capping layer. It has been found, that the gate electrode is most effective underneath a channel of comparable width, while the position of the gate electrode allows to shift the oscillations. Temperature and applied bias voltage in turn adjust the number of charge carriers in the system. Understanding the influences of the various parameters allows to precisely tailor the system's properties to the needs of future applications.

HL 84.3 Thu 15:30 H17

Highly Mismatched GaAs1-xNx and Ge1-xSnx Alloys Prepared by Ion Implantation and Ultrashort Annealing — •Shengqiang Zhou — Helmholtz-Zentrum Dresden Rossendorf, Dresden, Germany

Doping allows us to modify semiconductor materials for desired properties such as conductivity, bandgap, and/or lattice parameter. A small portion replacement of the highly mismatched isoelectronic dopants with the host atoms of a semiconductor can result in drastic variation of its structural, optical, and/or electronic properties. Here, the term 'mismatch' describes the properties of atom size, ionicity, and/or electronegativity. In this talk, we present the fabrication of two kinds of highly mismatched semiconductor alloys, i.e., Ge1-xSnx [1] and GaAs1-xNx [2]. The results suggest an efficient above-solubility doping induced by non-equilibrium methods of ion implantation and ultrashort annealing. Pulsed laser melting promotes the regrowth of monocrystalline Ge1-xSnx, whereas flash lamp annealing brings about the formation of high quality GaAs1-xNx with room temperature photoluminescence. The bandgap modification of Ge1-xSnx and GaAs1-xNx has been verified by optical measurements of spectroscopic ellipsometry and photoluminescence, respectively. In addition, effective defect engineering in GaAs has been achieved by flash lamp annealing, by which a quasi-temperature-stable photoluminescence at 1.3 um has been obtained [3, 4]. [1] K. Gao, et al., APL 105, 042107 (2014); [2] K. Gao, et al., APL 105, 012107 (2014); [3] K. Gao, et al., JAP 114, 093511 (2013); [4] S. Prucnal, et al., Opt. Express, 20, 26075 (2012).

HL 84.4 Thu 15:45 H17

Disentangling bulk from surface contributions in the electronic structure of black phosphorus — •Evangelos Golias, Maxim Krivenkov, and Jaime Sánchez-Barriga — Helmholtz-Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein Str. 15, 12489 Berlin, Germany

Most recently, black phosphorus (BP) has come into focus as a promising material for future applications in nanoelectronic devices due to its unique electronic and transport properties. Here, we use angle-resolved photoemission spectroscopy (ARPES) in conjunction with ab-initio calculations within the framework of density-functional theory (DFT) to disentangle surface from the bulk contributions in the electronic structure of BP. We find good agreement between our theoretical predictions for the intra and interlayer energy-momentum dispersions and the experimentally obtained three-dimensional band structure of this material. Our results provide compelling evidence for the existence of surface-resonant states near the top of the valence band which can play an important role in the performance of electronic devices based on BP.

30 min. Coffee Break

HL 84.5 Thu 16:30 H17

Optoelectronic and charge transport properties of Ta_3N_5 from first principles — •Juliana Morbec[1,2] and Giulia Galli[1] — [1]Institute for Molecular Engineering, University of Chicago, USA — [2]Department of Physics, University of Duisburg-Essen, Germany

Tantalum nitride (Ta_3N_5) is considered a promising material for photoelectrochemical water splitting due to its suitable band gap ($\sim$ 2.1 eV) for visible light absorption and favorable band-edge positions for water splitting. However, Ta_3N_5 photoanodes have been shown to exhibit poor performance, probably due to their rapid photodegradation and to limitations in their charge transport properties. Using first-principles calculations we carried out a detailed study of the optoelectronic and charge transport properties of crystalline Ta_3N_5 [1,2]. We present an analysis of the optoelectronic properties of Ta_3N_5 [1], showing that this material is highly anisotropic, with heavy holes in several directions, pointing to low mobilities. We also discuss the polaronic contributions to the hole and electron mobilities and the effect of stress and substitutional impurities on the electronic structure of Ta_3N_5 [2]. We show that the overall large effective masses of electrons and holes may be reduced with applied strain.
[1] Juliana M. Morbec, Ieva Narkeviciute, Thomas F. Jaramillo, and Giulia Galli, Phys. Rev. B 90, 155204 (2014).
[2] Juliana M. Morbec and Giulia Galli, 2015 (submitted).
ACKNOWLEDGMENTS: This work was supported by the National Science Foundation under the NSF Center CHE-1305124 for CCI Solar Fuels.

HL 84.6 Thu 16:45 H17

Assessment of first-principles structure optimisations, their impact on the band structures, and relative stability of polytypes in GaSe and InSe semiconductors — •Andrei Postnikov[1], Juliana Srour[1,2], Michael Badawi[1], and Fouad El Haj Hassan[2] — [1]Université de Lorraine, LCP-A2MC, Metz, France — [2]Université Libanaise, Faculté des Sciences, Beirut, Lebanon

Lattice parameters of β, γ, δ and ε polytypes of III-VI semiconductors GaSe and InSe are optimised in a sequence of first-principles (within the density functional theory) calculations, done with WIEN2k [1] and VASP [2] codes in comparison, the both being applied with a number of exchange-correlation (XC) "flavours". An underestimation of the van der Waals (vdW) gap between the Se-(cation)-(cation)-Se double layers is largely corrected by inclusion of the vdW interaction according to the (semiempirical) Grimme scheme. A critical analysis is done of different XC types in what regards their impact on the accuracy of the structure prediction and on the fine placement of the valence /

conduction bands. The band structures are discussed with respect to their relation to those in chalcopyrite-type $Cu(Ga,In)Se_2$ compounds [3] and in the hexagonal In_2Se_3. For both binary compounds studied, different polytypes are ordered according to their energetic preference.

1. The WIEN2k code, `http://www.wien2k.at` .
2. The VASP code, `http://www.vasp.at` .
3. J.Srour, M. Badawi, F. El Haj Hassan, and A. V. Postnikov, to be published in phys.stat.solidi (c).

HL 84.7 Thu 17:00 H17

Electronic structure calculations for carbon nanotubes under strain — •Christian Wagner[1,3], Jörg Schuster[2], Michael Schreiber[3], Andre Schleife[4], and Thomas Gessner[1,2] — [1]Center for Microtechnologies, TU Chemnitz, Germany — [2]Fraunhofer Institute ENAS, Chemnitz, Germany — [3]Institute of Physics, TU Chemnitz, Germany — [4]Department for Materials Science, University of Illinois at Urbana-Champaign, USA

Carbon nanotube (CNT) optics is an active field of research and is becoming increasingly interesting for applications. CNTs show unique properties upon strain: Under load, their band gap is opening or closing (depending on the CNTs' chirality) which makes them suitable for electronic and optical strain sensing at the nano scale. Further, they could operate as strain-tunable emitters.

We present results of electronic structure calculations for strained CNTs: we employ density functional theory (DFT) for ground states, GW approximation for a correct description of the fundamental gap, and we solve the Bethe-Salpeter-equation for the optical polarization function.

Our results are strain-dependent band gaps and the derived deformation potentials for different CNT chiralities. The strain-induced shift of exciton-related peaks is quantified. This requires cutting off the Coulomb interaction of periodic images in our supercell approach. The strain parameters derived here can be used for large-scale device modeling and is compared to available literature data.

HL 84.8 Thu 17:15 H17

Cubic scaling GW: towards fast quasiparticle calculations — •Peitao Liu[1,2], Merzuk Kaltak[1], Jiri Klimeš[1], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [2]Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

Within the framework of the full potential projector-augmented wave (PAW) methodology, we present a promising low scaling GW implemention. It allows for quasiparticle calculations with a scaling that is cubic in the system size and linear in the number of k points used to sample the Brillouin zone. This is achieved by calculating the independent particle polarizability in real space and imaginary time via contraction over the Green's functions of occupied and unoccupied states. The Fourier transformation of the polarizability from the imaginary time to frequency domain is done by a very efficient discrete Fourier transformation with only a few nonuniform grid points. Fast Fourier transformations are used to go from real space to reciprocal space and vice versa. The analytical continuation from the imaginary axis to the real axis is done by exploiting the Thiele's reciprocal difference method. Finally, the method is applied successfully to predict the quasiparticle energies and spectral functions of typical semiconductors (Si, SiC, GaAs and ZnO) and metals (Na, Al, Pd, and $SrVO_3$). The results are compared with conventional standard GW calculations. Good agreement is achieved, highlighting the power of this method.