HL 20: Poster IA (Ultrafast phenomena; Optical properties; Transport; Theory)

Presenters are kindly requested to be near their poster for at least one hour in the time between 17:00-19:00 or to leave a note about their availability for discussions.

Time: Monday 15:00–20:00 Location: Poster B

HL 20.1 Mon 15:00 Poster B

Laser induced Tellurium formation detected by THz oscillations in plasmonic crystals — •Jonas Vondran[1], Lars E. Kreilkamp[1], Martin Pohl[1], Maciej Wiater[2], Tomasz Wojtowicz[2], Grzegorz Karczewski[2], Boris. A Glavin[3], Leonid Litvin[4], Axel Rudzinski[4], Michael Kahl[4], Ilya A. Akimov[1,5], Dmitri R. Yakovlev[1,5], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland — [3]Lashkaryov Institute of Semiconductor Physics, 03028 Kyiv, Ukraine — [4]Raith GmbH, Konrad-Adenauer-Allee 8, 44263 Dortmund, Germany — [5]A. F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

We study the differential reflectivity of a CdMgTe structure in pump-probe experiments on a femtosecond timescale under below bandgap excitation. In the transient data oscillations with frequencies in the 3.6 - 3.8 THz range are observed. We attribute this to coherent oscillation of optical phonons in a thin Tellurium layer on the sample surface which is formed on the II-VI semiconductor due to a surface reconstruction induced by the pump beam. Changes in frequency and amplitude with increasing exposure time allow to monitor the build-up process of the Tellurium layer.

We show that the oscillatory signal is enhanced by one order of magnitude via patterning of a plasmonic grating with a period of several hundreds of nanometers.

HL 20.2 Mon 15:00 Poster B

Electron dynamics driven by light carrying orbital angular momentum — •Jonas Wätzel and Jamal Berakdar — Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle

The feasibility of light carrying orbital angular momentum (OAM) opened new opportunities in photonics [1] but also in optoelectronics. When interacting with matter, OAM beams may transfer a torque to the carrier with an amount governed by the topological charge l. This allows to steer the orbital [2] as well as the spin dynamics [3]. Indeed, an OAM beam irradiating an injected electronic wave packet in a 2D semiconductor stripe results in an edge charge-density accumulation that can be steered by the OAM beam [2].

Here, we present results for an isolated mesoscopic 2D ring driven by OAM laser. The calculations reveal that due to the transferred torque a directed current can be generated and controlled by the sign and the strength of the topological charge l. We also discuss technological applications of these phenomena.

[1] L. Allen, S. M. Barnett, and M. Padgett, Optical Angular Momentum (Institute of Physics Publishing, Bristol, 2003).

[2] J. Wätzel, A. S. Moskalenko and J. Berakdar, Opt. Express 20, 27992 (2012)

[3] G. F. Quinteiro and J. Berakdar, Opt. Express 17, 20465 (2009)

HL 20.3 Mon 15:00 Poster B

Ab-initio MD-simulations of the response of titanium dioxde after fs-laser exciation — •Sergej Krylow[1], Fairoja Cheenicode Kabeer[1,2], Eeuwe S. Zijlstra[1], and Martin E. Garcia[1] — [1]Theoretical Physics II, University of Kassel — [2]Theory Department, Fritz Haber Institute Berlin

The response of titanium dioxide was determined by using our in-house Code for Highly-excIted Valence Electron Systems(CHIVES), which is based on electronic temperature dependent density functional theory using pseudopotentials and localized atom-centered basis functions. We are especially interested in the decay of the A1g phonon mode as well as the phonon-phonon interaction causing this decay. We show that the dynamics of the decay is dependent on the applied fs-laser fluence and we comapre the result with recent experiments [1]

[1] E. M. Bothschafter , A. Paarmann , E. S. Zijlstra, N. Karpowicz, M. E. Garcia, and R. Ernstdorfer: Ultrafast evolution of the excited-state potential energy surface of TiO_2 single crystals induced by carrier cooling

HL 20.4 Mon 15:00 Poster B

Ultrafast carrier dynamics and coherent oscillations in PbTe — •Prashant Padmanabhan[1], Kestutis Budzinauskas[1], Kiran H. Prabhakara[1], Benoît Fauqué[2], Kamran Behnia[2], and Paul H. M. van Loosdrecht[1] — [1]Physics Institute 2, University of Cologne, 50937 Cologne, Germany — [2]LPEM (UPMC-CNRS), Ecole Supérieure de Physique et de Chimie Industrielles, 75005 Paris, France

PbTe is a leading thermoelectric material that, in addition to its low thermal conductivity, shows unusually large carrier mobilities at very low doping levels. Here, we report on ultrafast pump-probe experiments on PbTe that shed light on these, as of yet, ill-understood properties. By employing time-resolved differential reflectivity measurements, the dynamics of electron-electron and electron-phonon interactions on the femtosecond time-scale are studied. The influences of sample temperature and pump fluence on the time constants of the various scattering pathways are also investigated. In addition, our experiments have revealed the presence of coherent oscillations in the differential reflectivity with a frequency close to those associated with LA+TO excitations; these may provide a means to further study the giant anharmonic coupling that is central to the low thermal conductivity of PbTe.

HL 20.5 Mon 15:00 Poster B

Plasmon-Exciton coupling in stacked 2D Perovskite Semiconductors — •David Leipold[1], Wendy Niu[2], Lindsey Ibbotson[2], G. Vijaya Prakash[3], Jeremy J. Baumberg[2], and Erich Runge[1] — [1]Technische Universität Ilmenau, Germany — [2]University of Cambridge, UK — [3]Indian Institute of Technology Delhi, India

The coupling of plasmons and non-linear materials is a vital part in the developement of future plasmonic devices. Strong coupling and the formation of new plasmon-exiton quasiparticles called Excimons was previously observed in metal-semiconductor hybrid systems and organic dye coated metal-gratings. Here, we discuss $(C_6H_9C_2H_4NH_3)_2PbI_4$ (CHPI) as a candidate material for active plasmonic devices. In contrast to other materials, CHPI shows strong excitonic response and high stability even at room temperature. It can viably be processed from solution and forms regular stacks of semiconducting sheets. We present experiments and calculations for the optical properties of CHPI on nanostructured metal-gratings. We observe the formation of collective grating-exciton modes that are coupled with a Rabi splitting of 125-150meV. The role of the interaction of the CHPI exciton with its image-exciton in the metal is discussed as an additional interesting effect.

HL 20.6 Mon 15:00 Poster B

Surface plasmons at semiconductor/dielectric interfaces — •Dalibor Blažek[1,2], Michael Čada[2,1], and Jaromír Pištora[1] — [1]Nanotechnology Centre, VŠB - Technical University of Ostrava, 17. listopadu 15, Ostrava - Poruba, Czech republic — [2]Department of Electrical and Computer Engineering, Dalhousie University, Halifax, NS B3H 4R2, Canada

Plasmonic structures are a promising solution for developing novel integrated optics devices. While metals have shown to support plasmon oscillations at optical frequencies, heavily doped semiconductors may support surface plasmons (SP) at infrared frequencies. In order to fully understand the resulting SP characteristics, one needs to investigate properties of the lattice permittivity, the plasma frequency, and the damping.While these material properties may be regarded as the material constants, the relevant SP properties are dispersive. Focusing on the SP of a chosen wavelength, its characteristics may be tuned by a semiconductors doping level. While a minimum dopant concentration is required to support a chosen SP, as the doping concentrations increase, the secondary effects, such as decreasing electron mobility and increasing effective mass, will significantly affect plasmon damping.

This contribution presents the influence of doping levels on the SP properties. The calculations are based on the Drude model using the real semiconductor properties. It is shown that the propagation length of the SP increases monotonically with increasing doping levels despite the extremely large damping.

HL 20.7 Mon 15:00 Poster B

Control of Lasing from Bloch-States in Microcavity Photonic Wires via Selective Excitation and Gain — •Andreas Mischok[1], Robert Brückner[1], Alexander A. Zakhidov[1,2], Hartmut Fröb[1], Vadim G. Lyssenko[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden — [2]Texas State University, 601 University Drive, San Marcos, Texas, United States

Organic microcavities comprising the host:guest emitter system Alq_3:DCM offer an interesting playground to experimentally study the full dispersion characteristics of laterally patterned surface emitting lasers due to the broad emission spectrum and high quantum efficiency of the organic dye. By structuring directly on top of the bottom distributed Bragg reflector, we are able to precisely manipulate the mode structure and influence the coherent emission properties of the device. Adding SiO_2 photonic wire structures into an organic microcavity, we create an additional lateral confinement and a Bloch-like band-structure in the dispersion of periodically patterned cavities. We experimentally observe spontaneous and stimulated emission from the ground and different excited discrete states at room temperature. By changing the spatial gain distribution via a two beam interference, we are able to directly control the laser emission from both extended and confined modes of such organic photonic wires. Both spatial distribution and dispersion exhibit coherent emission from tunable modes, which we describe with an analytical model and numerical simulations, in perfect agreement with our measurements.

HL 20.8 Mon 15:00 Poster B

Towards coupling of photonic crystal cavities and waveguides as an integrated deterministic single-photon source in quantum photonic networks — •Stefan Hepp, Ulrich Rengstl, Matthias Paul, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Center for Integrated Quantum Science and Technology IQ^{ST}, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The generation and control of deterministic single photons is crucial for quantum photonic technologies like quantum teleportation, quantum computation and quantum cryptography. The requirements for such an on-demand single-photon source are a near unity photon-extraction and excitation efficiency coupled with a high degree of indistinguishability and an easy implementation in quantum photonic networks. Semiconductor quantum dots (QDs) have been proven as excellent candidates due to their outstanding optical properties and their easy integration in semiconductor nanophotonic devices. One main approach for an on-demand single-photon source is the positioning of QDs in photonic crystal cavities and waveguides for the coupling of the QD emission into guided modes, which is required for on-chip integration. An additional benefit of this approach is the exploitation of cavity quantum electrodynamic effects (cQED) to improve and manipulate the optical properties of the quantum dot emission. Here we present a way to an integrated on-demand single-photon source based on InAs/GaAs QDs positioned in a L3 photonic crystal cavity coupled to a waveguide for in-plane single-photon emission at 910nm.

HL 20.9 Mon 15:00 Poster B

Lasing Dynamics in ZnO & CdS Nanowires — •Marcel Wille[1], Tom Michalsky[1], Robert Röder[2], Carsten Ronning[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, 04103 Leipzig — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

The knowledge of the turning-on characteristic as well as of the laser dynamics itself is of great importance for the application of semiconductor nanowires (NWs) as on-chip integrated nanolaser. In this work we investigated the laser dynamics of high quality, CVD grown ZnO and CdS NWs using time-resolved micro photoluminescence technique. Experiments at room temperature clearly demonstrate the formation of an electron-hole plasma in both semiconductor materials accompanied by a spectral red shift of the PL emission as well as the drop of the decay constant above laser threshold. After the high exciting laser pulse the propagating NW laser modes exhibit a red shift in time, what can be explained with the increase of the refractive index with decreasing carrier density. Remarkably, modes closer to the excitonic energy exhibit a stronger red shift than lower energetic modes. In fact the modal shift depending on the initial mode energy is significantly higher in ZnO compared to CdS NWs.

HL 20.10 Mon 15:00 Poster B

Exciton polariton modes of a planar resonator in magnetic fields — •Steffen Richter, Chris Sturm, Helena Franke, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

Exciton-polaritons have gained large interest during the last years especially due to their ability to undergo Bose-Einstein-like condensation. Magnetic fields are important as they can be be used to control the polariton and resonator properties, e.g. in order to decrease condensation thresholds. Here, we show a theoretical study of the evolution of the polariton eigenmodes and their polarization properties (pseudo spin) in a planar resonator in the presence of a magnetic field. Thereby no restrictions of the direction of the magnetic field with respect to the polariton wave vectors are assumed. A 4×4 transfer matrix approach enables numerical application of the respective mode conditions with full polarization treatment at arbitrary in-plane wavevectors.

HL 20.11 Mon 15:00 Poster B

Temperature dependent dielectric function of hexagonal $YMnO_3$ — •Steffen Richter[1], Rüdiger Schmidt-Grund[1], Carsten Bundesmann[2], Stefan Ebbinghaus[3], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstr. 15, 04318 Leipzig, Germany — [3]Martin-Luther-Universität Halle-Wittenberg, Institut für Chemie, Kurt-Mothes-Str. 2, 06120 Halle, Germany

Rare earth manganites are promising due to the occurrence of multiferroic properties. Hexagonal $YMnO_3$ is ferrolectric up to high temperatures. Furthermore, it is antiferromagnetic below a Néel temperature of around 90K. Both features are coupled by the configuration of the manganese ions. In order to study a possible coupling to its optical properties we examine the uniaxial dielectric function of h-$YMnO_3$ in the NIR-VUV spectral range for temperatures from 10 to 300K. The measurements are performed at an *a*-plane oriented single crystal sample, grown by the optical floating zone technique. The temperature dependence of some Mn-related transitions gives hint to the occurence of a soft mode related to the antiferromagnetic phase transition.

HL 20.12 Mon 15:00 Poster B

Interference measurements on exciton-polariton Bose-Einstein Condensates — •Alexander Holm, Martin Thunert, Helena Franke, Chris Sturm, Tom Michalsky, Marius Grundmann, and Rüdiger Schmidt-Grund — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

We report on interference measurements to investigate the coherence properties of exciton-polariton Bose-Einstein condensates (BECs) in a ZnO-based planar microcavity at T = 10 K. The photoluminescence signal of the Fourier plane was sent to a Michelson interferometer in mirror-retroreflector (RR) configuration. The RR image is a centrosymmetric counterpart of the mirror arm image. In the resulting interferogram we superimpose the emission with opposite wavevectors.

By means of analyzing the fringe visibility of the interferogram as a function of the path length difference of both interferometer arms, a BEC coherence time at least (500 ± 200) fs could be deduced. This is about four times larger than the BEC lifetime demonstrating the coherence conservation during the multiple reabsorption and reemission process of this quantum system.

HL 20.13 Mon 15:00 Poster B

Impact of disorder on the coherence of a polariton condensate in dependence on the temperature — Martin Thunert[1], •Stefan Lange[1], Helena Franke[1], Chris Sturm[1], Alexander Janot[2], Bernd Rosenow[2], M. Dolores Martín[3], Luis Viña[3], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Uni Leipzig, Inst. für Exp. Physik II, Linnéstr. 5, 04103 Leipzig — [2]Uni Leipzig, Inst. für Theor. Physik, Brüderstr. 16, 04103 Leipzig — [3]Universidad Autónoma de Madrid, Departamento de Física de Materiales, C/ Francisco Tomás y Valiente, n* 7, 28049 Madrid, Spain

We report on the impact of disorder on the coherence proterties of an exciton-polariton Bose-Einstein condensate (BEC) in a ZnO-based bulk planar microcavity (MC). In general, disorder leads to reduced long-range correlations of the BEC, which may eventually result in frequency desynchronization or even in spatially separated condensate fragments. In our MC, the momentum space intensity distribution of the BEC emission is strongly affected by disorder even at high exci-

tation powers and for a wide range of temperatures and detunings. We found theoretically that this lack of BEC stabilization relies on the driven dissipative nature of the condensate, leading to disorder-induced density-independent phase fluctuations. We analyzed the interference pattern of the condensate emission pattern in momentum space for excitation powers slightly above the condensation threshold and a large range of temperatures up to 160 K. These measurements show that the emission from a certain energy state arises from a temporally coherent condensate rather than of uncorrelated BEC fragments.

HL 20.14 Mon 15:00 Poster B

Optical Properties of a Palladium-Tin Clusters as a Model System for Interfaces on a Molecular Scale — •Andre Rinn, Niklas Rinn, Stefanie Dehnen, and Sangam Chatterjee — Philipps-Universität Marburg, Germany

Palladium-containing compound-materials are of great interest for their catalytic properties. We have successfully grown a new Pd-Sn cluster with an organic shell which is a promising candidate for a next-generation heterogenic catalyst. From a more fundamental point of view, the interaction of the Pd and Sn core with the outer organic shell makes this cluster an interesting model system for internal interfaces on a molecular scale.

The compound crystalizes into micrometer-sized, well-ordered single-crystalline needles which are relatively ambient-insensitive. To characterize their optical response we perform linear absorption and steady-state PL under vacuum conditions in a microscopy setup containing all-reflective optics. Next, we study the transfer between the Pd-containing core and the outer shell for various excitation energies and fluencies to identify the charge-transfer mechanisms. Furthermore, the influence of different ambient conditions is investigated to explore surface adhesion effects on the optical response.

Financial support by the German Research foundation in the Framework of SFB 1083 is gratefully acknowledged.

HL 20.15 Mon 15:00 Poster B

Optical properties of organotin sulfide clusters — •Nils Rosemann[1], Jens Eussner[2], Stefanie Dehnen[2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Material Science Center, Philipps-Universität Marburg, Renthof 5,D-35032 Marburg, Germany — [2]Faculty of Chemistry and Material Science Center, Philipps-Universität Marburg, Hans-Meerweinstraße,D-35043 Marburg, Germany

Chalcogenide-based clusters offer a large variety of structural and physical properties which can be further functionalized by adding various different ligands. By changing the combination of cluster and ligand, their properties can be tuned to fit the desired purpose, e.g., optimized light harvesting in organic solar cells or enhancing the efficiency of electrolysis of water for hydrogen production. To identify the impact of different ligands, we study a series of three different organotin-sulfide clusters, based on the same core but with different functional groups. Only by changing the ligand, the optical properties change drastically, e.g., disabling optical activity or changing from optical activity to dichroism.

HL 20.16 Mon 15:00 Poster B

Time-resolved photoluminescence spectroscopy on silicon doped AlN, iron doped GaN and nominally undoped ZnO using correlational analysis — •Matthias Lamprecht[1], Benjamin Neuschl[1], Sebastian Bauer[1], Ramón Collazo[2], Martin Klein[3], Ferdinand Scholz[3], Zlatko Sitar[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany — [2]Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina 27606, USA — [3]Optoelectronics Department, University of Ulm, 89069 Ulm, Germany

We present results of time-resolved photoluminescence investigations using correlational analysis on a time scale of microseconds and milliseconds. Modulation of the pumping HeCd laser with a pseudorandom binary sequence yields correlational properties similar to white noise. Via cross correlation of the detected signal and the pseudorandom binary sequence the photoluminescence decay is computed. We applied this method to several defect-related photoluminescence bands in silicon doped AlN, iron doped GaN and nominally undoped ZnO and discuss the characteristics, and temperature dependencies.

HL 20.17 Mon 15:00 Poster B

Activated transport in nanoporous titanium dioxide under hydrogen exposure — •Sonja Allani[1], Thomas Heinzel[1], Mihai Cerchez[1], and Klaus Schierbaum[2] — [1]Solid State Physics Laboratory (IPkM), Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany — [2]Materials Science Laboratory (IPkM), Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

Nanoporous titanium dioxide is reduced to $TiO_{2-\delta}$ by thermal annealing. The oxygen vacancies act as donors and increase the conductivity. This material has been used for hydrogen sensing in the ppm range, [1] but the hydrogen-induced transport mechanism is not fully understood. Here, we present temperature dependent transport experiments of this material in the presence of atomic hydrogen. We observe a strongly decreasing conductivity as the temperature is decreased from 300 K to 40 K. The temperature dependence is consistent with both activated transport and variable range hopping within experimental uncertainties. Moreover, the current-voltage characteristics are nonlinear, incidating that reduced titanium dioxide does not become metallic under hydrogen exposure that is typical for sensing applications.

[1] M. Cerchez, H. Langer, M. El Achhab, T. Heinzel, D. Ostermann, H. Lüder, and J. Degenhardt, Appl. Phys. Lett. 103, 033522 (2013).

HL 20.18 Mon 15:00 Poster B

Asymmetric Hall cross junction — •Michael Szelong[1], Arne Ludwig[2], Andreas D. Wieck[2], and Ulrich Kunze[1] — [1]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum — [2]Angewandte Festkörperphysik, Ruhr-Universtät Bochum

We are analysing the influence of a geometrical asymmetry in a cross junction on Hall voltage in ballistic linear and nonlinear transport regime in a perpendicular magnetic field of up to 15 T. The cross junction consists of a straight current channel while two voltage probes merge into the middle of the current channel at an angle of 45°. All four emerging branches have the same length of 900 nm and the same width of 330 nm. A top-gate has not been processed to prevent threshold voltage shifts during measurements. The device has been processed on a high-mobility GaAs/AlGaAs heterostructure with a two-dimensional electron density of $n = 4.1 \cdot 10^{11}\mathrm{cm}^{-2}$ and a mobility of $\mu_n = 5.5 \cdot 10^5\mathrm{cm}^2/\mathrm{Vs}$, both at 4.2 K, resulting in an elastic mean free path of 5.8 μm.

A current through the current channel induces, with application of a perpendicular magnetic field, a Hall voltage in the 45-degree branches which is expected to be current polarity dependent, larger where electrons can easier enter the tilted branches, smaller in the opposite case. It is found that in non-linear regime this expectation is met whereas in weak non-linear regime it is sometimes turned upside down.

HL 20.19 Mon 15:00 Poster B

Hall effect in an asymmetric ballistic cross junction — •Joeren von Pock[1], Ulrich Wieser[1], Thomas Hackbarth[2], and Ulrich Kunze[1] — [1]Lehrstuhl für Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, D-44780 Bochum — [2]DaimlerChrysler Forschungszentrum Ulm, D-89081 Ulm

Low-temperature ($T = 4.2$ K) Hall measurements up to $B = 15$ T are performed on a ballistic cross junction consisting of 220 nm wide channels on a high mobility Si/SiGe heterostructure ($\mu_{2D} = 18.3\ \mathrm{m}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$, $n_{2D} = 6.3 \cdot 10^{15}\ \mathrm{m}^{-2}$ at 1.4 K). A non-centrosymmetric Hall geometry is formed by a straight current channel and oblique voltage probes attached to the channel under 45° in the same direction. A Pd gate electrode covers the whole structure. In the nonlinear transport regime (current $I \approx 1$ μA) at low magnetic fields ($B \leq 1$ T) the absolute value of the Hall voltage depends on the current direction [1]. This is explained in terms of ballistic cyclotron orbits propagating into the oblique probe channels. Surprisingly, the polarity dependence persists up to magnetic fields up to $B = 15$ T, where the cyclotron diameter shrinks to 13 nm, which is less than the effective channel width.

[1] U. Wieser *et al.*, Physica E **40**, 2179 (2008).

HL 20.20 Mon 15:00 Poster B

Hartree-Fock Ground State Phase Diagram of the Two-Dimensional Electron Gas with Spin-Orbit Interaction — •Akash Chakraborty, Paul Wenk, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

The two-dimensional electron gas (2DEG) has served as a prototype for the understanding of electrons in solid state and condensed matter physics, such as in the quasi two-dimensional semiconductor het-

erostructures. However, the quantum mechanical many-body nature of these systems increases the complexities and the Hartree-Fock (HF) approximation plays a fundamental role in tackling this problem. Starting from the early works of Overhauser[1], the HF ground state of the 2DEG has been studied over the years but the effects of spin-orbit interaction have not been studied extensively. We calculate the ground state of the 2DEG within the HF approximation in the presence of Rashba and Dresselhaus spin-orbit coupling. Based on an earlier work[2], which included only the Rashba term, we try to identify two competing phases, a ferromagnetic one with partial out-of-plane polarization and a paramagnetic one with in-plane spin. A phase diagram in terms of the electron density and the relative intensities of the spin-orbit couplings with respect to the Coulomb interaction is also presented.

[1] A. W. Overhauser, Phys. Rev. Lett. 4, 462 (1960); Phys. Rev. 128, 1437 (1962).

[2] L. O. Juri and P. I. Tamborenea, Phys. Rev. B 77, 233310 (2008).

HL 20.21 Mon 15:00 Poster B

Effect of B/N co-doping on optical properties of Graphene — •Pooja Goyal — Dep. of Physics, Panjab University, Chandigarh — DAV College Chandigarh

Ab-initio calculations based on density functional theory (DFT) have been performed to study the optical properties of pure graphene as compared BN co-doped graphene sheet. The effect of doping has been investigated by varying the concentrations of dopants from 6.25 % (one atom of the dopant in 32 host atoms) to 75 % for BN co-doping also varying the doping sites. The dielectric function has been calculated within the random phase approximation (RPA) using VASP (Vienna ab-initio Simulation Package) code. The dielectric function, absorption spectrum and energy loss-function of single layer graphene sheet have been calculated for light polarization parallel and perpendicular to the plane of graphene sheet and compared with doping graphene. The calculated dielectric functions and energy-loss spectra are in reasonable agreement with the available theoretical and experimental results. It has been found that there is significant red shift in absorption towards visible range of the radiation at high doping concentration. The results suggest further investigations in this direction for application of graphene in photonics in visible region of light.

HL 20.22 Mon 15:00 Poster B

***Ab-Initio* Studies of X-Ray Absorption in Kesterites** — •Archana Manoharan, Lorenzo Pardini, Karsten Hannewald, and Claudia Draxl — Humboldt-Universität zu Berlin, Institut für Physik und IRIS Adlershof, Zum Großen Windkanal 6, 12489 Berlin, Germany

The kesterite Cu_2ZnSnS_4 (CZTS) is considered as good absorber material for solar-cell applications because it contains only non-toxic and inexpensive metals. In the present work, we study the structural and electronic properties of CZTS using density-functional theory within the generalized gradient approximation (GGA-PBEsol). X-ray absorption spectra are obtained by solving the Bethe-Salpeter equation of many-body perturbation theory. We explore the sulfur K and $L_{2,3}$ edges in CZTS as well as in binary phases like ZnS etc. The *ab-initio* calculations are carried out by the all-electron full-potential code *exciting*. A detailed analysis of the observed spectral signatures is performed by comparison with available experimental data.