HL 12: 2D Materials I: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)

Time: Monday 10:30–13:45 Location: WIL C107

Invited Talk HL 12.1 Mon 10:30 WIL C107

A microscopic view of graphene quantum Hall edge states with STM and AFM measurements — •Joseph A. Stroscio — NIST, Gaithersburg, MD 20899, USA

2D heterostructed devices with electrostatic pn junction boundaries provide a convenient geometry for the examination of Quantum Hall edge states with microscopic probes. In this talk I will review our work in circular and rectangular geometries to examine the quantum Hall edge states which form in high magnetic field using scanning tunneling microscopy (STM) and atomic force microscopy (AFM) measurements. In circular graphene pn junctions a concentric series of compressible and incompressible rings form due to electron interactions, and show single electron charging when probed by scanning tunneling spectroscopy. In a rectangular Hall bar geometry defined by pn junction boundaries, the compressible strips form the topological protected edge states in the quantum Hall effect. For the graphene Hall bar device, we utilize simultaneous AFM, STM, and quantum transport measurements at mK temperatures. The Kelvin probe force microscopy (KPFM) mode of AFM detects the chemical potential transitions when Landau levels are being filled or emptied as a function of back gate potential. In particular, symmetry breaking states can be resolved at filling factors $\nu = *1$ inside the N=0 Landau level manifold, showing the lifting of the graphene four-fold degeneracy due to spin and valley. With KPFM we can map the dispersion of the Landau levels across the quantum Hall edge boundary as a function of density and spatial position, including resolving the $\nu = *1$ edge modes.

HL 12.2 Mon 11:00 WIL C107

Energy dissipation on suspended graphene quantum dots — •Alexina Ollier[1,2], Marcin Kisiel[1], Urs Gysin[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel,Klingelbergstr. 82, 4056 Basel, Switzerland — [2]Swiss Nanoscience Institute, Klingelbergstrasse 82, 4056 Basel

Here we report on a low temperature (T=5K) measurement of striking singlets or multiplets of dissipation peaks above graphene nanodrums surface. The stress present in the structure leads to formation of few nanometer sized graphene quantum dots ribbons (GQDRS) and the observed dissipation peaks are attributed to tip-induced charge state transitions in quantum-dot- like entities. The dissipation peaks strongly depend on the external magnetic field (B=0T-2T), the behavior we attributed to crossover from quantum dot carrier confinement to the confinement by magnetic field.

HL 12.3 Mon 11:15 WIL C107

The edge morphology and electronic properties of ballistic sidewall zig-zag graphene nanoribbons on SiC (0001) — •T.T.Nhung Nguyen[1], H. Karakachian[2], J. Aprojanz[1], U. Starke[2], A. Zakharov[3], C. Polley[3], and C. Tegenkamp[1] — [1]TU Chemnitz, Germany — [2]Max Planck Institute, Germany — [3]MAX IV Lab, Sweden

Epitaxial graphene nanoribbons grown on SiC(0001) mesa structures were shown to reveal ballistic transport at room temperature. The subsequent improvement of preparation parameters allows us to fabricate large scale zig-zag type ribbons with 40nm in widths with a pitch size down to 200 nm. We analyzed the electronic structure of the ribbons and their edges by ARPES and STM/STS. Indeed, ARPES reveals clearly the Dirac cone from the ribbon. The Fermi energy coincides with the Dirac point. This finding is corroborated by STS, revealing an elastic tunneling gap of around 130meV. STM shows that the zig-zag edge merges into the SiC substrate. Exactly at the position of this edge, a metallic state is seen at 0V. The gradual decrease of its intensity within 3nm comes along with a peak splitting. Moreover, the valence and conduction band states reveal close to the edge a larger gap of around 300 meV. We assign these findings to a hybridization of the zig-zag GNR edge with SiC. Furthermore, we propose that the ballistic transport is rather mediated by a 1D interface state rather than by a GNR edge state. The interface state mimics massive particles, which is consistent with the energy positions of electron transmission peaks found in GNR nanoconstrictions of various lengths.

HL 12.4 Mon 11:30 WIL C107

Attosecond-fast current control at graphene-based interfaces — •Tobias Boolakee, Christian Heide, Heiko B. Weber, and Peter Hommelhoff — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Epitaxially grown monolayer graphene on bulk n-doped silicon carbide (SiC) forms a Schottky contact with remarkable electronic and optical properties. We show that charge transfer across the graphene-SiC solid-state interface takes place within (300 ± 200) attoseconds ($1\ \text{as} = 10^{-18}$ s), which is the fastest charge transfer observed across a solid-state interface [1]. To reveal the attosecond dynamics, we apply femtosecond laser pulses and use saturable absorption in graphene as an intrinsic clock to determine how long an excited state stays excited before charge transfer and thermalization depopulate this state. Recent experimental results and a simple theoretical modelling based on rate equations and on a quantum mechanical model will be presented [2,3].

[1] Heide, C. et al. accepted in Nat. Photon.
[2] Higuchi, T. et al. Nature **550**, 224–228 (2017).
[3] Heide, C. et al. New J. Phys. **21** (2019).

HL 12.5 Mon 11:45 WIL C107

Sideband generation & pseudospin-flip excitations in graphene using tr-momentum microscopy — •Marius Keunecke[1], David Schmitt[1], Christina Möller[1], Davood Momeni Pakdehi[2], Hendrik Nolte[1], Wiebke Bennecke[1], Marie Gutberlet[1], Matthijs Jansen[1], Marcel Reutzel[1], Klaus Pierz[2], Daniel Steil[1], Hans Werner Schumacher[2], Sabine Steil[1], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen. I. Physikalisches Institut, 37077 Göttingen, Germany — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

The coherent control of quantum states is a promising route towards new emerging phases in solids. One of these phases are the so called Floquet-Bloch states, created by a periodic driving laser. Other light-matter coupled states (Volkov states) arise close to the surface of a solid and are understood as a final state dressing by the laser light. In graphene, the driving by circularly polarized light is predicted to open up a bandgap at the dirac point and thus creating a Floquet topological insulator [1]. In our experiment, the electronic bandstructure of ML graphene on SiC (0001) is mapped during photo-excitation using a momentum microscope in combination with a 1 Mhz femtosecond HHG lightsource (26.6 eV). Different pump wavelengths and polarizations are used to disentangle the excited states dynamics and the sideband generation at high momenta. We will discuss the nature of the generated sidebands and the photoinduced anisotropic hot carrier distributions. [1] M. A. Sentef et al., Nat. Commun. 6, 7047 (2015)

HL 12.6 Mon 12:00 WIL C107

Melting the low temperature gap in monolayer VSe_2, in time resolved ARPES — •Deepnarayan Biswas[1,2], Alfred Jones[1], Paulina Majchrzak[1,3], Klara Volckaert[1], Charlotte Sanders[1,3], Igor Marković[2], Federico Andreatta[1], Akhil Rajan[2], Yu Zhang[3], Gabriel Karras[3], Tsung-Han Lee[4], Chang-Jong Kang[4], Byoung Ki Choi[5], Richard Chapman[3], Adam Waytt[3], Emma Springate[3], Jill Miwa[1], Philip Hofmann[1], Phil D. C. King[2], Young Jun Chang[5], Nikola Lanata[1], and Søren Ulstrup[1] — [1]Aarhus University, Denmark — [2]University of St Andrews, UK — [3]Central Laser Facility, UK — [4]Rutgers University, USA — [5]University of Seoul, Republic of Korea

The group V transition metal dichalcogenide VSe_2 shows a charge density wave (CDW) transition at 110 K with $(4 \times 4 \times 3)$ charge ordering in its bulk form. In contrast, recent experiments on monolayer (ML) VSe_2 have shown an enhanced transition at $\sim$ 140 K with very different charge ordering. Moreover, this transition is accompanied by a full gapping of the Fermi surface. Here, we have used time and angle resolved photoelectron spectroscopy (TR-ARPES) to understand the electron dynamics in ML VSe_2 above and below the transition temperature. We have also modelled the ARPES intensity using a modified BCS self energy and density functional theory calculated bare bands. We find the gapped phase vanishes upon pumping and takes unusually long time to recover (more than 10 ps). This behaviour points toward a hot electron relaxation bottleneck coupled with an electronic phase transition in this sample.

HL 12.7 Mon 12:15 WIL C107

Time-dependent momentum distributions of bright and dark excitons in bulk WSe2 — •Shuo Dong[1], Samuel Beaulieu[1], Dominik Christiansen[2], Maciej Dendzik[1], Tommaso Pincelli[1], Rui Patrick Xian[1], Julian Maklar[1], Malte Selig[2], Andreas Knorr[2], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Transition metal dichalcogenide semiconductors feature exceptional optoelectronic properties. The investigation of excited states in k-space provides access to optically-bright and dark states on equal footing. Here, we perform the momentum-resolved excited-state mapping in the entire first Brillouin zone of bulk WSe2 using time-resolved momentum microscopy. Upon resonant excitation of band gap, the bright excitons with trARPES signal in the K valleys rapidly scatter to finite-momentum dark excitons in the Σ valleys. We analyze the shape and size of momentum distribution of the excited state. Under the plane wave final state approximation, the Fourier transform of photoemission signal yields real-space image of excitonic wave function. Combined with a microscopic theoretical description of exciton dynamics, the momentum-resolved valley carrier distribution provides information of fundamental exciton properties, like size, binding energy and exciton-phonon coupling.

HL 12.8 Mon 12:30 WIL C107

Sub-picosecond photo-induced displacive phase transition in two-dimensional $MoTe_2$ — •Bo Peng[1,2], Hao Zhang[2], Heyuan Zhu[2], Bartomeu Monserrat[1], and Desheng Fu[3] — [1]TCM Group, Cavendish Laboratory, University of Cambridge, United Kingdom — [2]Department of Optical Science and Engineering, Fudan University, China — [3]Department of Optoelectronics and Nanostructure Science, Shizuoka University, Japan

Photo-induced phase transitions (PIPTs) provide an ultrafast, energy-efficient way for precisely manipulating the topological properties of transition-metal ditellurides, and can be used to stabilize a topological phase in an otherwise semiconducting material. By first-principles calculations, we demonstrate that the PIPT in monolayer $MoTe_2$ from the semiconducting 2H phase to the topological 1T' phase can be driven purely by electronic excitations. The photo-induced electronic excitation changes the electron density, and softens the lattice vibrational modes. These pronounced softenings lead to structural symmetry breaking within sub-picosecond timescales, which is far shorter than the timescale of a thermally driven phase transition. The transition is predicted to be triggered by photons with energies over 1.96 eV, corresponding to an excited carrier density of 3.4×10^{14} cm^{-2}, which enables a controllable phase transformation by varying the laser wavelength. Our results provide insight into the underlying physics of the phase transition in 2D transition-metal ditellurides, and show an ultrafast phase transition mechanism for manipulation of the topological properties of 2D systems.

HL 12.9 Mon 12:45 WIL C107

Understanding electron beam damage in 2D materials from first-principles calculations: Effects of chemical etching and electronic excitation — •Silvan Kretschmer[1] and Arkady V. Krasheninnikov[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Applied Physics, Aalto University School of Science, Aalto, Finland

Two-dimensional (2D) materials are routinely characterized nowadays in the transmission electron microscope (TEM). The high-energy electron beam in TEM can create defects in the target, and as the influence of defects on materials properties is expected to be stronger in systems with reduced dimensionality, understanding defect production in 2D materials is of particular importance. Irradiation-induced defects can appear through three mechanisms, namely ballistic or knock-on damage (1), ionization and electronic excitations (2) and beam-induced chemical etching (3). Only the first channel is well understood, while observations of defects formation in 2D transition metal dichalcogenides below the knock-on threshold point out that other mechanism should be important. Here we investigate the role of beam-induced chemical etching and electronic excitations in defect production by using ab-initio molecular dynamic simulations and advanced first-principles simulation techniques based on the Ehrenfest dynamics combined with time-dependent density-functional theory. We demonstrate that the adsorption of small beam-induced radicals and electronic excitations dramatically lower the displacement threshold.

HL 12.10 Mon 13:00 WIL C107

Interaction of highly charged ions with single, bi- and trilayer graphene — •Anna Niggas[1], Janine Schwestka[1], Sascha Creutzburg[2], Benjamin Wöckinger[1], Tushar Gupta[3], Bernhard C. Bayer-Skoff[3], Friedrich Aumayr[1], and Richard A. Wilhelm[1,2] — [1]TU Wien, Institute of Applied Physics, Vienna, Austria — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [3]TU Wien, Institute of Materials Chemistry, Vienna, Austria

The interaction of highly charged ions (HCIs) with surfaces has been in the focus of many groups over the last decades. Recently, the rise of 2D materials has provided access to study the neutralisation dynamics of HCIs as they have not reached their equilibrium charge state inside atomically thin materials yet.

In our experiment, we use Xe ions (Xe^{1+} to Xe^{44+}) with energies in the range of 1-400 keV as projectiles and we then record the exit charge states of the ions after transmission through 2D materials. Additionally, we are able to determine the energy loss during the interaction through time of flight measurements, the yield and energy of emitted secondary electrons and forward sputtered target atoms in coincidence.

We now focus especially on the dependence of the neutralisation process on the thickness of the target. Thus, we employ single, bi- and trilayer graphene to mimic graphite with adjustable thickness. In order to ensure that this target structure is not affected by contaminations, it is crucial to implement cleaning procedures. Possible *in-situ* techniques and their effects will also be discussed in this context.

HL 12.11 Mon 13:15 WIL C107

Neutralization of ions transmitted through graphene and MoS_2 monolayers — •Sascha Creutzburg[1,7], Janine Schwestka[2], Anna Niggas[2], Heena Inani[3], Anthony George[4], Lukas Madauss[5], Stefan Facsko[1], Jani Kotakoski[3], Marika Schleberger[5], Andrey Turchanin[4], Pedro L. Grande[6], Friedrich Aumayr[2], and Richard A. Wilhelm[1,2] — [1]HZDR, Ion Beam Center, Dresden, Germany — [2]TU Wien, Institute of Applied Physics, Vienna, Austria — [3]University Vienna, Faculty of Physics, Vienna, Austria — [4]Friedrich Schiller University Jena, Institute of Physical Chemistry, Germany — [5]University Duisburg-Essen, Faculty of Physics and CENIDE, Germany — [6]Federal University of Rio Grande do Sul, Porto Alegre, Brazil — [7]TU Dresden, Germany

Ion irradiation is a widely used technique for material modification. The use of ion irradiation for defect engineering in 2D materials requires a high sensitivity of energy deposition in the surface during the ion's impact. Ions of high charge states (e.g. Xe^{30+}) deposit their potential energy of up to tens of keV in shallow surface depths triggering nanostructure formation. In fact, nanostructure formation in 2D materials, like carbon nanomembranes or MoS_2, due to the impact of Xe ions of charge states larger than 28 was observed. In contrast, no nanostructures on graphene were found, even after irradiation with Xe^{40+} ions. Here, we investigated the ion's neutralization during the transmission through freestanding graphene and MoS_2 monolayers. We deduce the lost energy of the ions (kinetic and potential) in experiment and put our results into context of nanostructuring.

HL 12.12 Mon 13:30 WIL C107

Ab-initio Exciton-polaritons: Cavity control of two-dimensional Materials — •Simone Latini[1], Enrico Ronca[1], Hannes Hübener[1], Umberto De Giovannini[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free Electron Laser Science, 22761 Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth avenue, New York NY 10010

We put forward a novel way of controlling the optical features of two-dimensional materials by embedding them in a cavity. The cavity light-matter interaction leads to the formation of exciton-polaritons, mixed states of matter and light. We demonstrate a reordering and mixing of bright and dark excitons leading to the direct optical observation of the latter. In type II van-der-Waals heterostructure, we show that the cavity provides control on the stabilization of inter- over intralayer excitons. Our theoretical predictions are based on a newly developed non-perturbative many-body framework that involves the ab-initio solution of the coupled quantized electron-photon Schrödinger equation in a quantum-electrodynamics plus Bethe-Salpeter approach. Within this framework we are able to investigate exciton-polariton

states and predict their dispersion and response in a strong cavity light-matter coupling regime. Our method lends itself to the investigation of more complex polaritonic, so called phonoriton, a mixture of excitons, phonons and photons. In particular we were able to identify elusive phonoritonic spectral features observed in a state-of-the-art pump and probe experiment.