

DS 30: Two-dimensional materials IV (jointly with HL/TT)

Time: Wednesday 9:30–13:15

Location: POT 51

DS 30.1 Wed 9:30 POT 51

Landau-Quantized Graphene: A Tunable Nonlinear Optical Material in the THz Range — ●JACOB C. KÖNIG-OTTO^{1,2}, YONGRUI WANG³, ALEXEY BELYANIN³, CLAIRE BERGER^{4,5}, WALT A. DE HEER⁴, MILAN ORLITA^{6,7}, ALEXEJ PASHKIN¹, HARALD SCHNEIDER¹, MANFRED HELM^{1,2}, and STEPHAN WINNERL¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf, Germany — ²Technische Universität Dresden, Germany — ³Texas AM University, USA — ⁴Georgia Institute of Technology, USA — ⁵CNRS-Université Alpes, France — ⁶LNCMI, Grenoble, France — ⁷Charles University in Prague, Czech Republic

Finding nonlinear optical materials for the THz and mid-infrared regimes is not straightforward. State-of-the-art devices with a high third-order optical susceptibility are often processed as complex multi-quantum-well structures designed to feature one specific resonance frequency. In our work we study Landau-quantized graphene as a tunable and simple to produce nonlinear material. To this end we perform time-integrated degenerate four-wave mixing (FWM) experiments at a photon energy of 78 meV resonant to the transitions between the Landau levels LL_{-1} , LL_0 and LL_1 at a magnetic field of roughly 4 T. We can recover expected scaling of the FWM-signal with the incident fields and the resonance behavior. The value of the third-order surface susceptibility in this material is in agreement with our calculations based on the density matrix formalism. We find the order of $\chi^{(3)}$ of Landau-quantized graphene to be competitive with more complex and elaborated solutions.

DS 30.2 Wed 9:45 POT 51

Ballistic transport in 2D periodically modulated graphene — ●ANDREAS SANDNER¹, MARTIN DRIENOVSKY¹, KENJI WATANABE², TAKASHI TANIGUCHI², DIETER WEISS¹, and JONATHAN EROMS¹ — ¹Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — ²NIMS, 1-1 Namiki, Tsukuba, Japan

Embedding graphene into a heterostructure with hexagonal boron nitride was shown to be an efficient way of achieving a high bulk mobility. The encapsulated graphene is protected in any further top-down fabrication procedure and pronounced commensurability features could be observed in 2D antidot lattices [1].

Here, we want to introduce a new method for periodical modulation of the carrier density, employing a few layer graphene patterned bottom gate. The bottom gate is defined by etching a 2D hole array into the few layer graphene and adapts perfectly to the commonly used stacking method for van der Waals heterostructures. By tuning the local bottom gate and the global back gate voltage, we can switch between the unipolar and bipolar transport regime.

We fabricated patterned bottom gates with lattice periods down to 150 nm and observe pronounced commensurability peaks that can be nicely compared to experiments with hard-wall graphene antidot lattices. We report on the difference between the unipolar and the bipolar regime, as well as the influence of the magnitude of the imposed superlattice potential.

[1] A. Sandner et al., Nano Lett. **15**, 8402 (2015)

DS 30.3 Wed 10:00 POT 51

Commensurability oscillations in electrostatically modulated graphene — ●MARTIN DRIENOVSKY¹, JONAS JOACHIMSMEYER¹, TAKASHI TANIGUCHI³, KENJI WATANABE³, MING-HAO LIU², KLAUS RICHTER², DIETER WEISS¹, and JONATHAN EROMS¹ — ¹Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — ²Institut für Theoretische Physik, Universität Regensburg, Germany — ³National Institute for Material Science, Tsukuba, Japan

We report on the first experimental observation of commensurability oscillations (COs) [1] in a 1D periodic graphene superlattice. Employing a locally acting few layer graphene patterned bottom gate (FLG PBG) and a dry van-der-Waals stacking method we prepare high mobility graphene-boron nitride heterostructures, where the ballistic length exceeds several periods of the modulation. The potential landscape can be tuned by the striped FLG PBG and a global back gate in such a way that a small, periodic and unipolar potential perturbation is generated. The magnetoresistance exhibits well pronounced COs at predicted magnetic field positions for electrostatic modulation, both for the electron and hole transport regime. Our measurements

confirm strong robustness of the COs in graphene with respect to temperature [2], as they remain visible up to 155 K.

[1] D. Weiss et al., Europhys. Lett. **8**, 179 (1989) [2] A. Matulis and F. M. Peeters, Phys. Rev. B **75**, 125429 (2007)

DS 30.4 Wed 10:15 POT 51

Intrinsic mobility due to electron-phonon interaction in black phosphorus. — ●SERGEY BRENER, ALEXANDER RUDENKO, and MIKHAIL KATSNELSON — Radboud Universiteit, Nederlanden

Flexural and in-plane thermal fluctuations in crystalline membranes affect the band structure of the carriers, which has an effect on transport properties of 2D systems. I consider a specific example of one-layer black phosphorus, which is a highly anisotropic material, and present our recent results on intrinsic carrier mobility. In contrast to graphene, where the mobility is determined by two-phonon (flexural) scattering, in black phosphorus one-phonon (in-plane) processes dominate.

DS 30.5 Wed 10:30 POT 51

Strain-induced commensurability oscillations in graphene — ●JONAS JOACHIMSMEYER¹, MARTIN DRIENOVSKY¹, TAKASHI TANIGUCHI², KENJI WATANABE², DIETER WEISS¹, and JONATHAN EROMS¹ — ¹Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — ²National Institute for Materials Science, Tsukuba, Japan

We realized a periodic strain modulation in a graphene/hexagonal boron-nitride (hBN) heterostructure by transferring it onto a prepatterned 1D superlattice etched into hBN. The transfer was performed using a dry van-der-Waals pick-up technique. This method yields a high mobility graphene device with a mean free path exceeding the period of the corrugation.

We conducted magnetotransport experiments in this corrugated graphene monolayer with a period of 150 nm. The modulation leads to a periodic strain which in turn gives rise to an effective periodic pseudopotential with half of the period of the corrugation [1], i.e. 75 nm. Due to the periodic potential we observe commensurability oscillations (COs) [2] in the longitudinal magnetoresistance, however superimposed by Shubnikov-de Haas (SdH) oscillations. Since both oscillations show different temperature dependences we increased the temperature up to 80 K. While the SdH oscillations get suppressed the COs still remain visible.

[1] Burgos, R., and Lewenkopf, C., arXiv:1610.04068 (preprint 2016).

[2] Ye, P. D., Weiss, D., et al., Semicond. Sci. Technol. **10**, 715 (1995).

DS 30.6 Wed 10:45 POT 51

Temperature switchable type of conductivity in hybrid conjugated polyelectrolyte/graphene two-dimensional nanocomposites — ●VIKTOR BRUS¹, MARC GLUBA¹, CHENG-KANG MAI², STEFANY FRONK², JÖRG RAPPICH¹, NORBERT NICKEL¹, and CUIILLERMO BAZAN² — ¹Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany — ²Center for Polymers and Organic Solids, Department of Chemistry and Biochemistry, University of California at Santa Barbara, Santa Barbara, CA, 93106, USA

We found that a submonolayer of CPE-PyrBI_m4 on CVD-grown graphene forms a novel two-dimensional hybrid material that exhibits preferential transport of holes or electrons as a function of temperature. Doping efficiencies increase with the increase of the temperature used to anneal the heterobilayers and a decrease of the CPE-PyrBI_m4 film thickness. The switching of the conductivity type of the thin CPE-PyrBI_m4/graphene heterobilayer composite occurs when graphene is not strongly overcompensated. Moreover, the conversion of the conductivity type is reversible. Doping mechanisms under consideration include charge transfer from electron rich structural units in the CPE-PyrBI_m4 backbone and/or field-effect doping as a result of interfacial electrostatic effects from adjacent ionic functionalities. This effect shows the unique and complex nature of electrical properties of the novel heterobilayer hybrid organic-inorganic CPE-PyrBI_m4/graphene nanocomposite material and enhances interest in further investigations.

DS 30.7 Wed 11:00 POT 51

Interlayer screening in n-doped bilayer and trilayer transition metal dichalcogenides — ●ANDOR KORMÁNYOS¹, VIKTOR ZÓLYOMI², and GUIDO BURKARD¹ — ¹University of Konstanz, Germany — ²Manchester University, United Kingdom

We derive an effective Hamiltonian based on the k.p approach that describes the dispersion at the band edges of the conduction band of bilayer and trilayer transition metal dichalcogenides (TMDCs). This model is then used to consider n-doped bilayer MoS₂ placed in uniform external electric field. We discuss the charge re-distribution between the layers due to the electric field and calculate the bandgap that opens at the K-point of the Brillouin zone in self-consistent Hartree approximation. We point out the relation between the induced band-gap and the quantum capacitance and briefly discuss the relevance of our results to recent photoluminescence experiments in double gated bilayer MoS₂.

Coffee Break

DS 30.8 Wed 11:45 POT 51

Driven Hofstadter Butterflies — ●MARTIN WACKERL¹ and JOHN SCHLIEMANN² — ¹Institut für Theoretische Physik, Universität Regensburg — ²Institut für Theoretische Physik, Universität Regensburg

Periodically driven quantum systems offer a great way of tuning band structures or Chern numbers. The first part will be about graphene illuminated with circular polarized light. The external driving is introduced via the Floquet formalism and the main focus will be on the deformation of the band structure of graphene. Afterwards we will give a short introduction to the Hofstadter butterfly and unify it with the Floquet formalism. We will show how the Hofstadter spectrum gets distorted when tuning the light intensity, photon energy, and polarization. The last part is about the influence of polarized light to the distribution of ground state Chern numbers of the Floquet-Hofstadter spectrum.

DS 30.9 Wed 12:00 POT 51

Resonant scattering off adatoms in monolayer graphene — ●SUSANNE IRMER, DENIS KOCHAN, and JAROSLAV FABIAN — University of Regensburg, Regensburg, Germany

We present a theoretical investigation of resonant scattering off adatoms on graphene. Resonant scattering is an important feature of adatoms as it leads to resonant enhancement of the impact of proximity effects such as local magnetic moments or spin-orbit coupling [1,2,3]. We investigate the three different adsorption positions of hollow, top, and bridge employing effective realistic tight-binding models and the T-matrix formalism. The developed resonance conditions are useful for quantum transport models as well as studies of spin relaxation in graphene with adatoms.

This work was supported by the DFG SFB 689 and GRK 1570, and by the European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] D. Kochan, M. Gmitra, and J. Fabian, Phys. Rev. Lett. 112, 116602 (2014)

[2] J. Bundesmann, D. Kochan, F. Tkatschenko, J. Fabian, and K. Richter, Phys. Rev. B 92, 081403 (2015)

[3] D. Kochan, S. Irmer, and J. Fabian, arXiv:1610.08794

DS 30.10 Wed 12:15 POT 51

Experimental realization and characterization of an electronic Lieb lattice — ●MARLOU SLOT¹, THOMAS GARDENIER¹, PETER JACOBSE¹, GUIDO VAN MIERT², SANDER KEMPKES², STEPHAN ZEVENHUIZEN¹, CRISTIANE MORAIS SMITH², DANIEL VANMAEKELBERGH¹, and INGMAR SWART¹ — ¹Debye Institute for Nanomaterials Science, Utrecht University, Netherlands — ²Institute for Theoretical Physics, Utrecht University, Netherlands

Geometry, whether on the atomic or nanoscale, is a key factor for the electronic band structure of materials. For example, the honeycomb geometry leads to Dirac-type bands where the charge carriers behave as massless particles. Theoretical predictions are triggering the exploration of novel 2D geometries, such as graphynes, Kagomé and the Lieb lattice. The latter is the 2D analogue of the 3D lattice exhibited by perovskites; it is a square-depleted lattice, which is characterised by a band structure featuring Dirac cones intersected by a topological flat band. Whereas photonic and cold-atom Lieb lattices have been demonstrated, an electronic equivalent in 2D is difficult to realize in an existing material. Here, we report an electronic Lieb lattice formed by the surface state electrons of Cu(111) confined by an array of CO molecules positioned with a scanning tunneling microscope. Us-

ing scanning tunneling spectroscopy and wave-function mapping, we confirm the characteristic electronic structure of the Lieb lattice. The experimental findings are corroborated by muffin-tin and tight-binding calculations. At higher energy, second-order electronic patterns are observed, which are equivalent to a super-Lieb lattice.

DS 30.11 Wed 12:30 POT 51

Interlayer Configuration in Twisted Bilayers of Folded Graphene — ●JOHANNES C. RODE, CHRISTOPHER BELKE, HENNRİK SCHMIDT, and ROLF J. HAUG — Institut für Festkörperphysik, Leibniz Universität Hannover

Twisted bilayer graphene (TBG), i.e. stacks of two graphene sheets in arbitrary rotational misalignment, exhibit rich electronic spectra[1,2] which are highly dependent on the interlayer twist angle in general[3] as well as details in stacking configuration like lattice commensuration and corrugation[4] in particular. We here examine the latter TBG properties coming from the morphological side: TBG are prepared via Atomic Force Microscope, folding ribbons out of monolayer sheets. In the recently proposed picture of a thermally activated growth process[5], here measured quantities like interlayer distance and shape of the folded edge are found to hold novel information about angle-dependent interlayer configuration and provide insight about interaction in van der Waals bound materials.

[1] H. Schmidt; J. C. Rode; D. Smirnov; R. J. Haug, Nat. Comm. 5, 5742 (2014).

[2] J. C. Rode; D. Smirnov; H. Schmidt, R. J. Haug, 2D Materials 3, 035005 (2016).

[3] J. M. B. Lopes dos Santos; N. M. R. Perez; A. H. Castro Neto, Phys. Rev. Lett. 99, 25682 (2007).

[4] E. J. Mele, Phys. Rev. B 81, 161405(R) (2010).

[5] J. Annett; G. L. W. Cross, Nature 535, 271-275 (2016).

DS 30.12 Wed 12:45 POT 51

Multi-scale approach for strain-engineering of phosphorene — DANIEL MIDTVEDT¹ and ●ALEXANDER CROY² — ¹Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — ²Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany

A multi-scale approach for the theoretical description of deformed phosphorene is presented. This approach combines a recently developed valence-force model [1] to relate macroscopic strain to microscopic displacements of atoms and a tight-binding model [2] with distance-dependent hopping parameters to obtain electronic properties. The resulting self-consistent electromechanical model is suitable for large-scale modeling of phosphorene devices. We demonstrate this for the case of an inhomogeneously deformed phosphorene drum, which may be used as an exciton funnel [3].

[1] D. Midtvedt and A. Croy, Phys. Chem. Chem. Phys. 18, 23312 (2016). [2] A. N. Rudenko, S. Yuan, and M. I. Katsnelson, Phys. Rev. B 92, 085419 (2015). [3] P. San-Jose et al, Phys. Rev. X 6, 031046 (2016).

DS 30.13 Wed 13:00 POT 51

Evolution of electronic structure of few-layer phosphorene from angle-resolved photoemission spectroscopy of black phosphorous — ●NIELS EHLEN¹, BORIS SENKOVSKIY¹, ALEXANDER FEDOROV^{1,2,3}, ANDREA PERUCCHI⁴, PAOLA DI PIETRO⁴, ANTONIO SANNA⁵, GIANNI PROFETA⁶, LUCA PETACCIA⁴, and ALEXANDER GRÜNEIS¹ — ¹Institute of Physics II, University of Cologne, Germany — ²IFW Dresden, Germany — ³St. Petersburg State University, Russia — ⁴Elettra Sincrotrone Trieste, Italy — ⁵Max Planck Institute of Microstructure Physics, Halle, Germany — ⁶Department of Physical and Chemical Sciences/SPIN-CNR, University of L'Aquila, Italy

A complete set of tight-binding parameters for the description of the quasiparticle dispersion relations of black phosphorous (BP) and N -layer phosphorene with $N = 1 \dots \infty$ is presented. The parameters, which describe valence and conduction bands, are fit to angle-resolved photoemission spectroscopy (ARPES) data of pristine and lithium doped BP. We show that zone-folding of the experimental three-dimensional electronic band structure of BP is a simple and intuitive method to obtain the layer-dependent two-dimensional electronic structure of few-layer phosphorene. Zone-folding yields the band gap of N -layer phosphorene in excellent quantitative agreement to experiments and *ab-initio* calculations. A combined analysis of optical absorption and ARPES spectra of pristine and doped BP are used to estimate a value for the exciton binding energy of BP.