

CPP 29: Two-dimensional Materials II: graphene (joint session HL/CPP)

Time: Tuesday 14:00–15:45

Location: H36

CPP 29.1 Tue 14:00 H36

Field-controllable spin relaxation anisotropy in graphene/hBN heterostructures — ●KLAUS ZOLLNER¹, MARTIN GMITRA², and JAROSLAV FABIAN¹ — ¹Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — ²Institute of Physics, P. J. Šafárik University in Košice, 04001 Košice, Slovakia

Measurements show a large and tunable anisotropy in the spin relaxation of hBN encapsulated bilayer graphene [1,2], similar to what is observed in graphene/TMDC heterostructures [3]. Combining systematic first principles calculations for graphene/hBN heterostructures with a minimal tight-binding model, we extract spin-orbit coupling parameters of graphene in the μeV range. The extracted model parameters depend on (i) interlayer distances, (ii) stacking configurations, and (iii) an external electric field, resulting in a rich parameter space. Based on the Dyakonov-Perel formalism we calculate spin relaxation times for graphene, in the nanosecond range, in agreement with recent experimental measurements. A very important finding is that the spin relaxation anisotropy is maximum close to the charge neutrality point, decreasing with the doping level. In addition, we also show that the anisotropy can be tuned by means of an external electric field, via the precise control of the Rashba SOC.

This work is supported by the DFG SPP 1666.

- [1] Xu et al., PRL 121, 127703 (2018)
 [2] Leutenantsmeyer et al., PRL 121, 127702 (2018)
 [3] Cummings et al., PRL 119, 206601 (2017)

CPP 29.2 Tue 14:15 H36

Microscopic theory of band gap opening and spin-orbit splitting in graphene/TMDC heterobilayers — ●ALESSANDRO DAVID¹, ANDOR KORMÁNYOS², and GUIDO BURKAD¹ — ¹Department of Physics, University of Konstanz, Konstanz, Germany — ²Department of Physics of Complex Systems, Eötvös Loránd University, Budapest, Hungary

Bilayers of graphene and monolayer transition metal dichalcogenides (TMDCs) are fascinating van der Waals heterostructures with an interesting electronic band structure. Theoretical ab initio calculations have shown a gap opening and a spin-orbit splitting in the band structure of graphene that are induced by the TMDC layer [1, 2]. These results have been experimentally confirmed by recent magnetotransport experiments showing weak antilocalisation (WAL) [2, 3]. Using perturbation theory, we propose a microscopic model to explain the origin of the gap and of the spin-orbit splitting. We also consider the dependence of the spin-orbit splitting on the misalignment of graphene and TMDC layers.

[1] M. Gmitra, D. Kochan, P. Högl, and J. Fabian, Phys. Rev. B 93, 155104 (2016). [2] Z. Wang, D.-K. Ki, H. Chen, H. Berger, A. H. MacDonald, and A. F. Morpurgo, Nat. Comm. 6, 8339 (2015). [3] T. Wakamura, F. Reale, P. Palczynski, S. Guéron, C. Mattevi, and H. Bouchiat, Phys. Rev. Lett. 120, 106802 (2018).

CPP 29.3 Tue 14:30 H36

Spatio-temporal dynamics in graphene — ●ROLAND JAGO, SAMUEL BREM, and ERMIN MALIC — Chalmers University of Technology, Gothenburg, Sweden

While the time- and energy resolved non-equilibrium dynamics in graphene is well understood [1], there is only little known about spatio-temporal electron dynamics. Optically excited carriers at the interfaces of inhomogeneities (e.g. p-n junctions, different substrate regions) create density and temperature gradients resulting in diffusion of carriers. Since many-particle interactions and diffusion depend on the conditions of the inhomogeneity, the transport of carriers is asymmetric and results in a photocurrent.

In this work, we apply the density matrix formalism solving the spatio-temporal graphene Bloch equations. We provide microscopic access to time-, momentum and spatially resolved optical excitation, Coulomb- and phonon-induced relaxation dynamics, and conversion of light into electrical current in graphene. The gained microscopic insights allow us to predict optimal conditions for photodetection in graphene.

[1] E. Malic and A. Knorr, Ultrafast optics and relaxation dynamics, VCH-Wiley, Berlin (2013)

CPP 29.4 Tue 14:45 H36

How Laser-induced defects modify optical properties of semiconducting Armchair Graphene Nanoribbons — ●SEYED KHALIL ALAVI^{1,2}, BORIS V. SENKOVSKIY³, MARKUS PFEIFFER¹, DANNY HABERER⁴, FELIX R. FISCHER⁴, ALEXANDER GRÜNEIS³, and KLAS LINDFORS¹ — ¹Department of Chemistry, Universität zu Köln, Luxemburger Str. 116, 50939 Köln, Germany — ²Institut für Angewandte Physik der Universität Bonn, Wegeler Strasse 8, 53115 Bonn, Germany — ³II. Physikalisches Institut, Universität zu Köln, Zùlpicher Strasse 77, 50937 Köln, Germany — ⁴Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Armchair graphene nanoribbons (AGNRs) with tunable band gap are promising candidate for optoelectronic devices. We have earlier shown how photoluminescence emission is boosted via formation of laser-induced defects in AGNRs lattices [1]. Here we probe the origin of this modification by measuring the extinction spectrum of a layer of AGNRs. Our results show that there are two pronounced peaks at approximately 2.4 and 1.8 eV in the spectrum of pristine GNRs. The latter peak energetically coincides with emission feature. This peak surprisingly disappears from the extinction spectrum after defects formation. We thus attribute the 1.8 eV peak to a quenching state. We additionally extract the absolute absorbance of AGNRs and find that it is a factor of three higher than graphene absorbance in visible range. [1] B. V. Senkovskiy, M. Pfeiffer, S. K. Alavi, et al., Nano Lett. 17, 4029-4037, 2017.

CPP 29.5 Tue 15:00 H36

Anisotropic strain induces a transition between rhombohedral and Bernal stacking in multilayer graphene flakes — FABIAN GEISENHOF¹, RAÚL GUERRO-AVILES², MARTA PELC², FELIX WINTERER¹, TOBIAS GOKUS³, YASIN DURMAZ^{3,4}, DANIELA PRIESACK¹, JAKOB LENZ¹, FRITZ KEILMANN^{4,5}, ANDRES AYUELA², and ●THOMAS WEITZ^{1,4,5,6} — ¹AG Physics of Nanosystems, Faculty of Physics, LMU München, Germany — ²Donostia International Physics Center, San Sebastian, Spain — ³Neaspec GmbH, München, Germany — ⁴Department of Physics, LMU München, Germany — ⁵Center for Nanoscience (CeNS), München, Germany — ⁶Nanosystems Initiative Munich (NIM), München, Germany

Graphene multilayers are still full of surprises - this is clear at latest since the recent discovery of unconventional superconductivity in 'magic-angle' bilayer graphene. Not only in bilayers the density of states critically depends on the lateral alignment of subsequent layers, but also in thicker graphene stacks (e.g. in trilayers). There, two different forms of stacking, so called Bernal and rhombohedral stacking exist, each with distinct charge transport properties. Via combined theoretical and experimental efforts we have surprisingly found [1], that during the fabrication process with conventional e-beam lithography, anisotropic strain forces rhombohedrally stacked regions towards Bernal stacking. We have experimentally identified the stacking change with Raman spectroscopy and s-SNOM measurements and devised methods how to avoid the transformation. [1] F.G. Geisenhof et al. ArXiv:1810.00067 (2018)

CPP 29.6 Tue 15:15 H36

Bio-compatible graphene exfoliation assisted by flavin mononucleotide sodium: a molecular dynamics study — ●SHIRONG HUANG¹, ALEXANDER CROY¹, VIKTOR BEZUGLY^{1,2}, and GIANAURELIO CUNIBERTI^{1,3} — ¹Institute for Materials Science and Max Bergmann Center for Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — ²Life Science Inkubator Sachsen GmbH & Co. KG, Tatzberg 47, 01307 Dresden, Germany — ³Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, German

Flavin mononucleotide sodium (FMNS) was reported as a highly efficient bio-dispersant for the exfoliation of aqueous dispersions of defect-free, few-layer graphene flakes. Most importantly, FMNS is innocuous and environment friendly and can facilitate bio-medical applications of graphene. Although there is some experimental work on graphene exfoliation assisted by FMNS, it is not clear how FMNS molecules behave on the graphene flake. Here, we clarify the interaction between FMNS and graphene flakes via all-atom molecular dynamic simulations. The exfoliation mechanism of FMNS on the graphene flake is

investigated by the potential of mean force (PMF) of pairs of graphene flakes coated with FMNS. This work provides a basis for understanding of graphene exfoliation assisted by FMNS-like surfactants and paves a path to design highly efficient dispersants for defect-free, few layer graphene.

CPP 29.7 Tue 15:30 H36

Scanning Nitrogen-Vacancy Center Magnetic Imaging of Graphene Devices — •SUSANNE BAUMANN, ALEC JENKINS, SIMON MEYNELL, HAOXIN ZHOU, ANDREA YOUNG, and ANIA BLESZYNSKI

JAYICH — UC Santa Barbara, Santa Barbara, USA

The NV center is a quantum probe that is sensitive to a variety of fields (magnetic, electric, thermal, strain), can achieve nanoscale spatial resolution, is non-invasive, and can operate over a wide range of temperatures; hence it is an ideal tool for studying novel phases of matter that often emerge only below a critical temperature. Here we use a cryogenic scanning NV magnetometer to probe the stray magnetic field of a current running through a single layer graphene device. With this technique we are able to probe different regimes of current flow via their local signatures over a variety of temperatures.