TT 11: Graphene -Spin-Orbit Interaction (jointly with DS,HL,MA,O)

Time: Monday 11:30–13:45 Location: H17

TT 11.1 Mon 11:30 H17

Impurity-induced spin relaxation time in graphene from first principles — •Dmitry Fedorov[1], Martin Gradhand[2], Sergey Ostanin[1], Igor Maznichenko[3], Arthur Ernst[1], Jaroslav Fabian[4], and Ingrid Mertig[3,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom — [3]Martin-Luther-Universität Halle, Institut für Physik, 06099 Halle, Germany — [4]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

The spin relaxation time of conduction electrons in graphene caused by carbon and silicon impurities is studied by means of our *ab initio* approach, which was recently developed for bulk systems [1] and adapted now for the film geometry. It is found that both the momentum and spin relaxation times are extremely sensitive to the position of the impurities. We show that adatoms provide spin-flip rates 4 to 5 orders of magnitude larger than in-plane impurities. Our results strongly support the adatom-induced extrinsic mechanism of the experimentally observed spin relaxation in graphene [2].

[1] M. Gradhand et al., PRB 81, 020403(R) (2010)
[2] N. Tombros et al., Nature 448, 571 (2007)

TT 11.2 Mon 11:45 H17

D'yakonov-Perel' spin dephasing in single and bilayer graphene and the role of contact resistance on the spin dephasing time — Frank Volmer[1,2], Marc Drögeler[1,2], Eva Maynicke[1,2], •Nils von den Driesch[1,2], Tsung-Yeh Yang[1,2], Gernot Güntherodt[1,2], and Bernd Beschoten[1,2] — [1]II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]JARA: Fundamentals of Future Information Technology, 52074 Aachen, Germany

We investigate spin transport in both single and bilayer graphene nonlocal spin-valve devices. Similar to our previous studies on bilayer graphene [1], we observe an inverse dependence of the spin dephasing time on the carrier mobility in our single layer devices indicating the importance of D'yakonov-Perel' like spin dephasing in exfoliated single and bilayer samples.

This general trend is only observed in devices with large contact resistances (>1 kΩ). In contrast, the spin dephasing time is significantly reduced in samples with low ohmic contacts for both single and bilayer graphene indicating that an additional spin dephasing occurs underneath the spin injection and detection electrodes.

This work has been supported by DFG through FOR 912.

[1] T.-Y. Yang *et al.* Phys. Rev. Lett. **107**, 047206 (2011)

TT 11.3 Mon 12:00 H17

Intrinsic and substrate induced spin-orbit interaction in chirally stacked trilayer graphene — •Andor Kormanyos and Guido Burkard — University of Konstanz

We present a combined group-theoretical and tight-binding approach to calculate the intrinsic spin-orbit coupling (SOC) in ABC stacked trilayer graphene. We find that compared to monolayer graphene, a larger set of d orbitals (in particular the d_{z^2} orbital) needs to be taken into account. We also consider the intrinsic SOC in bilayer graphene, because the comparison between our tight-binding bilayer results and the density functional computations allows us to estimate the values of the trilayer SOC parameters as well. We also discuss the situation when a substrate or adatoms induce strong SOC in only one of the layers of bilayer or ABC trilayer graphene. Both for the case of intrinsic and externally induced SOC we derive effective Hamiltonians which describe the low-energy spin-orbit physics. We find that at the K point of the Brillouin zone the effect of Bychkov-Rashba type SOC is suppressed in bilayer and ABC trilayer graphene compared to monolayer graphene.

The the combination of group-theoretical and tight-binding approaches can be used to study the spin-orbit interaction in other quasi-two dimensional materials, such as MoS_2, as well.

TT 11.4 Mon 12:15 H17

Long Electron Spin Lifetimes in Armchair Graphene Nanoribbons — •Matthias Droth and Guido Burkard — University of Konstanz, 78457 Konstanz

Armchair graphene nanoribbons (aGNR) are promising as a host material for electron spin qubits because of their potential for scalability and long coherence times [1]. The spin lifetime T_1 is limited by spin relaxation, where the Zeeman energy is absorbed by lattice vibrations [2], mediated by spin-orbit and electron-phonon coupling. We have calculated T_1 by treating all couplings analytically and find that T_1 can be in the range of seconds for several reasons: (i) Van Vleck cancellation; (ii) weak spin-orbit coupling; (iii) low phonon density; (iv) vanishing coupling to out-of-plane modes due to the electronic structure of the aGNR. Owing to the vanishing nuclear spin of ^{12}C , T_1 is a good measure for overall coherence. These results and recent advances in the controlled production of graphene nanoribbons [3] make this system interesting for classical and quantum spintronics applications.

[1] B. Trauzettel *et al.*, Nature Phys. **3**, 192-196 (2007).
[2] M. Droth and G. Burkard, Phys. Rev. B **84**, 155404 (2011).
[3] X. Zhang *et al.*, arXiv:1205.3516 (2012).

TT 11.5 Mon 12:30 H17

Tunneling-induced Spin Anisotropy Barrier in Quantum Dot Spin-Valves — •Michael Hell[1,2], Maciej Misiorny[1,2], and Maarten Wegewijs[1,2,3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich — [2]JARA - Fundamentals of Future Information Technology — [3]Institut für die Theorie der Statistischen Physik, RWTH Aachen, 52056 Aachen

Spintronics employs the two fundamental properties of a each electron: its charge and its spin-dipole moment. However, recent studies indicate that the interplay of these two degrees of freedom does not exhaust the potential of spintronics when approaching the nano-scale: spin correlations between electrons, partly characterized by the spin-anisotropy, provide an independent resource of spin information, which is stored even in a simple ferromagnet and couples to the spin-dipole moment in quantum dots. The interest in spin anisotropy also emerges from the research on single-molecule magnets (SMMs) and magnetic adatoms, in which the transport is controlled by a large spin anisotropy barrier intrinsically generated by strong spin-orbit coupling. In this talk we show that such a spin-anisotropy barrier can be externally induced by the transport of spin-correlations from ferromagnets into a a spin-isotropic interacting quantum dot with large spin S>1/2 and negligible spin-orbit interaction. This proximity-induced spin-anisotropy has the hallmarks of a spintronic exchange-field of a quadrupolar nature, a generalization of the well-established dipolar exchange field. The barrier increases with the tunnel coupling, achieving values comparable to that of SMMs, but with the flexibility of electric and magnetic tuneability.

TT 11.6 Mon 12:45 H17

First-principles study of the spin-orbit interaction in graphene induced by hydrogen adatoms — •Martin Gmitra, Denis Kochan, and Jaroslav Fabian — University of Regensburg

We have performed first principles calculations of the spin-orbit coupling effects in hydrogenated graphene structures, for varying hydrogen coverage densities, using the linearized augmented plane wave method as implemented in the FLEUR code. The covalent bonding between the hydrogen and carbon atoms leads to a local structural puckering of graphene sheets, giving rise to an overlap between the Dirac and sigma electrons and a giant enhancement (from roughly 0.01 to 1 meV) of the local spin-orbit interaction. The calculated effects on the band structure and the emerging spin patterns of the electronic states can be well explained by effective Hamiltonian models derived from group theoretical principles.

This work is supported by the DFG SPP 1285, SFB 689, and GRK 1570.

TT 11.7 Mon 13:00 H17

Theory of the hydrogen adatoms induced spin-orbit coupling in graphene — •Denis Kochan, Martin Gmitra, and Jaroslav Fabian — University Regensburg

We have analyzed the first-principles data of the electronic structure of hydrogenation in graphene by means of group theory derived effective Hamiltonians. We propose effective models for semihydrogenated graphene as well as for graphene with a single hydrogen adatom. The chemisorption of hydrogen modifies the structural symmetry of the

plane graphene in two essential ways—it breaks the pseudospin (sublattice) symmetry and induces rippling. We show that in addition to the Rashba spin-orbit interaction there emerges another spin-orbit field which is induced by the pseudospin inversion asymmetry due to the adatoms. Our realistic effective Hamiltonians should be useful for spin transport and spin relaxation investigations.

This work is supported by DFG SFB689

TT 11.8 Mon 13:15 H17

Optical properties of hydrogenated graphene from first principles — •Sebastian Putz, Martin Gmitra, and Jaroslav Fabian — Universität Regensburg, Universitätsstraße 31, 93053 Regensburg

We investigate the effect of hydrogen coverage on the optical properties of single-side hydrogenated graphene from first principles. To account for different degrees of uniform hydrogen coverage we calculate the complex dielectric function for graphene supercells of various size, each containing a single additional H atom. We use the Linearized Augmented Planewave (LAPW) method, as implemented in WIEN2k, to show that the hydrogen coverage strongly influences the complex dielectric function and thus the optical properties of hydrogenated graphene. The absorption coefficient in the visible range, for example, has different characteristic features depending on the hydrogen coverage. This opens up new possibilities of determining the hydrogen coverage of hydrogenated graphene samples in the experiment by contact-free optical absorption measurements.

This work is supported by the DFG GRK 1570.

TT 11.9 Mon 13:30 H17

Electron scattering and spin polarization at the graphene/Ni(111) interface — Aran Garcia-Lekue[1], Timofey Balashov[2], Marc Ollé[2], Gustavo Ceballos[2], Andrés Arnau[1,3], Pietro Gambardella[2], Daniel Sánchez-Portal[1,3], and •Aitor Mugarza[2] — [1]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 San Sebastian, Spain — [2]Catalan Institute of Nanotecnology (ICN), UAB Campus, E-08193 Bellaterra, Spain — [3]Centro de Fisica de Materiales CFM - MPC, Centro Mixto CSIC-UPV, Apdo. 1072, San Sebastian, Spain

The interaction of graphene with a metal often perturbs the unique electronic properties of Dirac electrons in graphene. This interaction can be positively exploited to engineer the Dirac bands and obtained graphene interfaces with different functionalities. In this work we study the electronic properties of graphene nanoislands grown on Ni(111) [1] by combining scanning tunnelling microscopy and ab-initio calculations. We show that the interaction with the Ni surface opens a gap and spin-polarizes the Dirac bands, which results in a spin filtering effect in the transport across the interface [2]. On the other hand, the standing wave pattern created around the nanoislands reveal an asymmetric potential that depends both on the spin and edge type, suggesting a lateral 2D spin-filter effect similar to that occurring across the interface.

[1] M. Olle et al. Nano Lett. 12, 4431 (2012). [2] V. M. Karpan et al. Phys. Rev. Lett. 99, 176602 (2007).