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

The spin relaxation time of conductors 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)
3. D’yakonov-Perel’ spin dephasing in single and bilayer graphene and the role of contact resistance on the spin dephasing time — Frank Volmer, Martin Gradhand, Eva Mayrnick, Nils von den Driesch, Tsung-Yeh Yang, Gernot Gütterbock, and Bernd Beschoten — Inst. of Physics, RWTH Aachen University, 52074 Aachen, Germany — JARA — Fundamentals of Future Information Technology, 52074 Aachen, Germany

We investigate spin transport in both single and bilayer graphene non-local 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.


Intrinsic and substrate induced spin-orbit interaction in chirally stacked trilayer graphene — Andor Kormányos 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_{3z^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 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 MoS₂, as well.

plane graphene in two essential ways—it breaks the pseudospin (sub-lattice) 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.

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.