TT 60: Graphene - Theory (jointly with DS, HL, MA, and O)

Time: Thursday 15:00–17:30 Location: H17

TT 60.1 Thu 15:00 H17

Influence of non-local exchange-correlation and spin-orbit interaction on electronic and optical properties of graphene, silicene, germanene, and tinene — •Lars Matthes[1], Olivia Pulci[2], Paola Gori[3], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Dipartimento di Fisica, Università di Roma "Tor Vergata", via della Ricerca Scientifica 1, 00133 Rome, Italy — [3]CNR-ISM, Via Fosso del Cavaliere 100, 00133 Rome, Italy

We present first-principles studies of the optical absorbance of the group-IV honeycomb crystals graphene, silicene, germanene, and tinene. We account for many-body effects on the optical properties by using the non-local hybrid functional HSE06. The optical absorption peaks are blue-shifted due to quasi-particle corrections, while the influence on the low-frequency absorbance remains unchanged and reduces to the universal value $\pi\alpha$,[1,2] where α is the Sommerfeld fine-structure constant. However, in silicene, germanene and tinene an electronic band gap arises at the Dirac-point due to spin-orbit splitting and parabolic bands with a very small effective mass emerge. Consequently, the low-frequency absorbance is modified due to the spin-orbit induced fundamental absorption edge. We demonstrate numerically that the absorbance increases at the fundamental absorption edge.

[1] A. Geim et al., Science 320, 1308 (2008)

[2] F. Bechstedt, L. Matthes et al., Appl. Phys. Lett. 100, 261906 (2012)

TT 60.2 Thu 15:15 H17

Generalized Hubbard models for two dimensional hybrid materials — •M. Rösner[1], E. Sasioglu[2], C. Friedrich[2], S. Blügel[2], A. I. Lichtenstein[3], M. I. Katsnelson[4], and T. O. Wehling[1] — [1]Institut für Theoretische Physik, Universität Bremen, D-28359 Bremen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]1. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [4]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands

We present effective generalized Hubbard models for the description of novel two dimensional materials. The local and non-local partially screened Coulomb interaction as well as hopping integrals are calculated from first principles for silicene and graphene on a metallic substrate. We consider interactions up to the 6th nearest neighbor in real space and investigate the long range behavior of the dielectric function in k-space. We compare the resulting silicene Hubbard model to the corresponding model for pure graphene. Thereby we find values of $U/t \approx 4.0$ eV for the on-site and $V/t \approx 2.4$ eV for the nearest neighbor partially screened Coulomb interaction in silicene, which are slightly bigger than in freestanding graphene. We further show that the ratio of the local to the non-local Coulomb interaction can be controlled by a metallic substrate, which efficiently screens non-local Coulomb terms.

TT 60.3 Thu 15:30 H17

Subgap conductivity in gated bilayer graphene — •Maxim Trushin — University of Konstanz, 78457 Konstanz

In the present work [1], the subgap electron transport has been investigated in gated bilayer graphene [2] within the two-band effective model using the finite-size Kubo formula. The conductivity does not vanish even though the temperature is set to zero and the chemical potential gets into the middle of the band gap. In contrast to the universal subgap conductivity observed in the 2D topological insulators [3], the subgap conductivity in bilayer graphene turns out to be sensitive to the band gap size and disorder strength.

The effect can be explained in terms of the quantum mechanical interband coherence which turns out to be important for the chiral carriers. At finite temperature, a competition between the temperature-dependent interband decoherence and thermal activation processes results in the non-monotonic conductivity vs. temperature dependence. The non-monotonicity can be seen as a signature of the interband entanglement responsible for the difference between the transport and spectral gaps. The effect can be observed in gapped bilayer graphene sandwiched in boron nitride where the electron-hole puddles and flexural phonons are strongly suppressed.

[1] M. Trushin, Europhys. Lett. **98**, 47007 (2012). [2] E. McCann, Phys. Rev. B **74**, 161403 (2006). [3] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).

TT 60.4 Thu 15:45 H17

Lattice dynamics of few-layer graphene after ultrashort laser excitation — •Naira Grigoryan, Eeuwe S. Zijlstra, and Martin E. Garcia — Universität Kassel, Kassel, Germany

Femtosecond laser pulses may induce striking structural effects in solids via electronic excitation. Here we studied the phonon dynamics on the 10 ps timescale in thin graphite films as a function of its thickness after laser interaction using ab initio molecular dynamics simulations including a Van der Waals force correction term to the local density approximation. We implemented the coupling of the hot electrons with the so-called strongly coupled optical phonons (SCOPs) [T. Kampfrath et al., PRL 95, 187403 (2005)] in a semiempirical way . From our simulations we could determine the decay of the SCOPs into other phonon modes, in particular, the out-of-plane lattice vibrations.

TT 60.5 Thu 16:00 H17

RKKY Interaction in a Graphene Bilayer — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

RKKY interaction in doped graphene monolayer ($k_F \neq 0$) shows Friedel oscillations decaying as $1/r^2$ [1]. In this work we consider the RKKY interaction in AA- and AB-stacked bilayer graphene using exact low energy Green's functions. Apart from the common site-to-site interaction we discuss impurities located at the bond centers as well as impurities at the center of the hexagonal plaquettes and intercalant-type impurities located in-between the two carbon layers. Similarly to the monolayer case, we find an oscillatory $1/r^2$ decay for on-site impurities in AA-stacked bilayer graphene. The exchange integral separates into the product of an energy dependent oscillation and an additional modulation resulting from the interlayer coupling. Interestingly, for on-site impurities in AB-stacked bilayer graphene this additional modulation vanishes at low Fermi energies. Moreover, due to the interference of the neighboring site-to-site interactions, at high Fermi energies the RKKY interaction between two plaquette impurities shows a $1/r^3$ behavior.

[1] M. Sherafati and S. Satpathy, Phys. Rev. B 84, 125416, 2011

Coffee break

TT 60.6 Thu 16:30 H17

***Ab initio* calculations of functionalized graphene nanoribbons** — •Christian Till, Nils Rosenkranz, Christian Thomsen, and Janina Maultzsch — TU Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, 10623 Berlin

Since nearly 30 years the discovery and subsequent research on fullerenes, carbon nanotubes, and graphene fuel expectations on carbon-based nanoelectronics. In this context, thin stripes of the two-dimensional material graphene, so-called graphene nanoribbons (GNRs), draw broad interest as well. In this work, we present a comprehensive ab initio study of the structural, electronic and vibrational characteristics of a 7-armchair GNR with hydroxyl functionalized edges. Our results show AGNRs with increasing hydroxyl saturation to be particularly stable. In addition, we find a variation of the ribbon geometry under functionalization. An increasing degree of functionalization leads to a compression perpendicular to the ribbon axis. As a consequence we find a linear shift of the band gap with growing edge hydroxylation. With regard to a possible experimental determination of the degree of functionalization, we indicate fingerprint vibrational modes of the hydroxyl groups as well as a substantial shift of Raman active phonons.

N. Rosenkranz, C. Till, C. Thomsen, and J. Maultzsch, Phys. Rev. B **84**, 195438 (2011).

TT 60.7 Thu 16:45 H17

Phonon dispersions of AB- and ABC-stacked graphene trilay-

ers and multilayers — •Bart Verberck[1,2], Karl H. Michel[1], and Björn Trauzettel[2] — [1]Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Recently, it was experimentally confirmed that the electronic structure of graphene multilayers crucially depends on how they are stacked. The simplest multilayer for which different stackings can be realised is the trilayer. The ABA variant features both linearly and quadratically dispersed electronic bands near the K-point, while the ABC variant has cubic electronic dispersion. At the same time, the difference between the phonon dispersions for ABA and ABC trilayer graphene is less well established. Detailed knowledge of the phonon spectra is, however, essential for understanding double-resonant Raman scattering experiments, offering a simple means for characterising multilayer graphene samples (number of layers and stacking sequence). Here we present a theoretical study of the phonon dispersions of AB- and ABC-stacked multilayers based on a phenomenological force-constants model. We find that the difference between the phonon spectra for the two variants is much less apparent than the difference between the respective electronic band structures; the main distinction concerns the low-energy phonon modes around the K-point. We argue that the observed difference in double-resonant Raman scattering signals for ABA and ABC trilayers mainly originates from the different electronic dispersions.

TT 60.8 Thu 17:00 H17

Optical selection rules in graphene quantum dots — •Eleftheria Kavousanaki and Keshav Dani — Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology, Graduate University, Okinawa, Japan

We theoretically study the optical absorption of graphene quantum dots for different shapes, sizes and edge types. We calculate the single particle energy spectrum using the tight-binding Hamiltonian and the Dirac-Weyl equation and show that dots with zigzag edges exhibit a degenerate shell of zero energy states, in agreement with previous results. Using standard group theoretical tools, we identify the optical selection rules for triangular and hexagonal quantum dots and discuss the role of light polarization on the absorption spectrum. Finally, we calculate the oscillator strengths and absorption spectra for different quantum dot sizes and identify the contribution of the zero energy states therein.

TT 60.9 Thu 17:15 H17

Electronic reflection for a single layer graphene quantum well — •Abir Mhamdi[1,2], Emna Ben Salem[1], and Sihem Jaziri[3] — [1]Laboratoire de Physique de la Matière Condensée, Faculté des Sciences de Tunis, Tunisia — [2]Institut für Theoretische Physik, Georg-August Universität Göttingen, Germany — [3]Laboratoire de Physique des Matériaux, Faculté des Sciences de Bizerte, Tunisia

We address the problem of Dirac fermions' graphene quantum well (GQW) and we focus on the low energy approximation for the Hamiltonian of the system where the former can be described by a Dirac-like Hamiltonian. Interesting relations are obtained and used to discuss the influence of the spin-orbit coupling, which induces an effective mass-like term, on the transport properties of single-layer graphene quantum well. It is found that the reflection probability of incident electrons is sensitive to the effective mass-like term. This can be explained by the dependence of reflection coefficient R on the incident electrons' direction and their energies. Notably, we found that the reflection probability for massive fermions with a very small angle, i.e. the wave-vector along the transport direction is zero in the GQW, can be greatly suppressed.