**Title: Determining the decisive spin**

**Abstract:** The Kondo effect caused in a metallic carbon nanotube by a transition metal impurity atom will influence electron transport, leading to potentially important zero bias anomalies in the nanotube conductance. The magnitude of the Kondo temperatures and the Fano conductance line shapes to be expected are presently unknown. We explore this problem at the first principles atomic level, specializing to Co (S=1/2) and Fe (S=1) impurities adsorbed alternatively outside or inside (4,4) and (8,8) single wall nanotubes. The principle zero bias anomalies, tiny and radius independent in the outside case, turn large and strongly radius dependent inside the nanotube, where the symmetry of the magnetic orbital changes from parallel to transverse to the tube axis, and thus hybridization is enhanced by a surrounding effect. These results foresee an interesting field and temperature dependence conductance, to be addressed in future experiments.

**References:**
Bo Gao

Gate controlled linear magneto-resistance in thin Bi2Se3 films

We report magnetoresistance data gained from thin Bi2Se3 films under the action of a back gate voltage. Upon application of high negative gate voltages, the sheets display linear magneto-resistance (LMR) for applied magnetic fields of a few Tesla. Under this condition, charge carriers in the bulk conduction band are depleted, such that the transport characteristic is mainly governed by the surface state. On this basis, we propose a parallel magneto-resistance model of the bulk MR and a quadratic B-field dependence of the bulk MR. This model accounts well for the observed thermally activated behavior of the bulk carrier density. In addition, we demonstrate that Abrinkosov's quantum magneto-resistance model [1] is well suited to explain both the the slope of LMR and the surface carrier density. These findings establish a novel tool to probe the Dirac surface state in topological insulators, even in the presence of pronounced disorder in the samples.


Benjamin Göhler

Spin Selectivity in Electron Transmission Through Self-Asssembled Monolayers of Double-Stranded DNA

In electron-transfer processes, normally spin effects are seen either in magnetic materials or in systems containing heavy atoms that facilitate spin-orbit coupling. Electron dichroism, namely different interactions of spin-polarized electrons with chiral molecules, has been reported for vortices of various chiral molecules. Polarized electron beams are attenuated differently, depending on the helicity of the electrons and the enantiomer of the molecules. In the gas phase this asymmetry of attenuation has been determined to be in the order of 10^-4 [1].


Rafael Gutierrez

Spin selective transport through helical molecular systems

Highly spin selective transport of electrons through a helically shaped electrostatic potential is demonstrated in the frame of a minimal model approach. The effect is significant even in the case of weak spin-orbit coupling. Two main factors determine the selectivity, an unconventional Rashba-like spin-orbit interaction, reflecting the helical symmetry of the system, and a weakly dispersive electronic band of the helical system. The weak electronic coupling, associated with the small dispersion, leads to a low mobility of the charge in the the system and allows for spin-orbit interactions to be effective. The results are expected to be generic for chiral molecular systems displaying low spin-orbit coupling and low conductivity.

Michael Hell

Spin-multipoletronics: quadrupolar exchange field and transport of spin anisotropy in quantum dot spin-valves

The spin anisotropy of a nanostructure is quantified by its spin-quadrupole and higher moments. While in spintronics setups involving states with spin > 1/2 the spin-quadrupole moment has to be treated as a addition of degree of freedom besides charge and spin, this provides a novel link between the fields of nanoscale spintronics and molecular magnetism. Such spin-anisotropy transport is of increasing importance when devices exhibiting spin-polarized currents approach the nanoscale where high spin states are stabilized by Coulomb and exchange interactions. To illustrate the basic idea we consider the simplified physical situation: an interacting single orbital that is exchange coupled to another impurity spin 1/2, resulting in a spin 1 quantum dot. We show that – in addition to charge and spin --- spin-quadrupole moment is transported when this high-spin quantum dot is tunnel-coupled to voltage-biased spin-polarized electrodes.

We develop a network theory by identifying the effective sources and current operators for spin-multipole transport quantities and derive their continuity equations. The transport of spin-anisotropy is shown to be radically different from that of spin and charge due to its multi-particle (multi-spin) nature. We furthermore find that the charge, spin and spin-quadrupole moment can accumulate and thereby influence each other whenever the quantum dot has accessible high-spin states (spin > 1/2) and non-equilibrium transport and / or quantum-fluctuation processes are important.

For the example considered we have extended the stationary kinetic equations for the charge and spin-multipole components of the density operator obtained in [1,2] to include transport processes of both leading order and next-to-leading order 2 in the tunnel coupling and arbitrary non-collinear spin-polarizations of the ferromagnets. We find new spin-induced effects, among which a tunneling of spin-anisotropy, analogous to spin and charge injection. Moreover, we systematically extract the coherent contributions to the time evolution induced by quantum fluctuations, recovering the dipolar exchange field [3] (coupacting to the quantum dot spin-dipole moment), which was demonstrated to be electrically tunable in a carbon nanotube spin-valve [4]. We illustrate how this effect is significant even in the case of a quadrupolar exchange field that couples to the spin-quadrupole moment thereby influencing the spin-dipole and charge accumulations in a new way: it gives rise to a spin-anisotropy barrier similar to that found in single molecule magnets, which is however externally induced and therefore under electric control.


George Japaridze

Spin and charge dynamics in a 1D correlated electron system with modulated spin-orbit interaction

We study the effect of spatially modulated Rashba spin-orbit interaction on the low-energy dynamics of a one-dimensionally correlated electron system with uniform, Rashba plus Dresselhaus, spin-orbits of the wave number of the modulation, commensurate with different diameters of the, characterized by four Fermi point Fermi surface of the system. We show that a spatially modulated Rashba spin-orbit coupling drives a transitions a) from a Luttinger liquid (LL) to an band-insulating (BI) state and b) from a metallic to a Helical liquid (HL) state.

Using an effective theory framework, we also carry out an analysis of effects from electron-electron interactions. In the case of LL-BI transition we show how the single-particle gap in the insulating state can be extracted from the more easily accessible collective charge and spin excitation thresholds and also give estimation for enhancement of the gap caused by e-e interaction. In the case of LL-HL transition, we give estimation for strength of the e-e interaction, at which gap opens for one-half of the conducting modes corresponding to the opposite spin orientations.


Aan Kaiser

Electronic conduction in different graphene samples and comparison with carbon nanotubes

The extraordinarily high mobility of electrons that is possible in graphene monolayers (away from the Dirac point) is limited at higher temperatures by scattering by phonons. Interestingly, the key role appears to be played by phonons of energy around 160 meV, as for single-wall carbon nanotubes (SWCNT) [1]. At low temperatures, the conductance in mesoscopic graphene samples often shows an anomalous increase or decrease that changes the sign of the applied gate voltage [2]. This is due to anomalies arise from “universal” mesoscopic resistive fluctuations, which extend to much higher temperature in graphene than in conventional 2D electron systems and decay exponentially (a feature that does not appear to be fully understood theoretically). We point out a remarkable analogy between electronic conduction in graphene prepared by chemical-vapour deposition [3], in reduced graphene oxide sheets [4], and in SWCNT films [5]. In each case, thermally-assisted conduction dominates but with a metal-like term at low temperatures; we can model the conduction in terms of the morphology of disorder in the samples.


Jens Kunstmann

Graphene edge magnetism for spintronics applications: Dream or Reality?

Graphene edge magnetism for spintronics applications: Dream or Reality?
The abstract of the oral presentation:We critically discuss the stability of edge states and edge magnetism in zigzag graphene nanoribbons (ZGNRs). We point out that magnetic edge states might not exist in real systems, and show that there are at least three very natural mechanisms – edge reconstruction, edge passivation, and edge closure – which dramatically reduce the effect of edge states in ZGNRs or even totally eliminate them. Even if systems with magnetic edge states could be made, the intrinsic magnetism would not be stable at room temperature. Charge doping destabilizes the intrinsic magnetism of such systems. We conclude that edge magnetism within graphene ZGNRs is much too weak to be of practical significance, in particular for spintronics applications. We further discuss the influence of nonmagnetic edges on the electron transport through ZGNRs.

References


Lucia Lenz

Dirac electrons in a periodic spin-orbit

We present a study of the band structure of Dirac electrons in graphene in the presence of one-dimensional, periodically modulated spin-orbit interactions. Based on the knowledge of the transfer matrix, we obtain an analytic equation for the...
potential band condition using the transfer matrix method. We investigate how the band structure changes compared to potentials with no spin-orbit interactions and its dependence on the length of the potential compared with the spin precession length.

Lakhapatt Lin Aigu

89% Positive Magnetoresistance in PANI-NP organic hybrid composite device with room temperature magnetoresistance of 89%, several times higher than the best reported values for organic-based devices. The device is also able to maintain its resistive state even when the power is switched off, thus exhibiting a memory effect.

Angel Mañanes

Magnetic properties of iron nanowires inside finite zigzag carbon nanotubes from first principles

We investigate the magnetic properties of iron nanowires encapsulated on carbon nanotubes (CNTs), performing “ab initio” calculations based on density functional theory using the ADF code. We consider an elongated (icosahedron) of Fe 12 located inside two different finite pieces of single walled zigzag carbon nanotubes (ZNTs) of indexes (10,0) and (11,0). We present the structure and magnetic properties of the Fe cluster-ZNT composites compared with those of the isolated systems. The properties of isolated ZNTs have been analyzed elsewhere [1]. The elongated structure found as a local minimum for Fe 12 presents a strong ferromagnetic coupling with total spin S=19. The magnetic moment per atom is smaller than for the free atoms, but larger than the corresponding to bulk iron. The electronic structure has a large electronic gap for the majority spin of 0.82 eV, and a much lower one for the minority spin, 0.09 eV. The minority spin presents a large density of states around the Fermi level.

When the iron aggregate interacts with the nanotubes it distorts slightly from its free geometry, and its optimal position inside the tube is not at the tube axis but close to the carbon wall. We found a decrement in the total magnetic moment: from S=19 in the free Fe 12 to S=18 in the combined systems, Fe12@(11,0) and Fe12@(10,0). Even if it can’t be an enhancement on the magnetic properties with respect to those of the isolated iron cluster, the interaction of the iron aggregate with the carbon nanotube preserves the strong ferromagnetic coupling of the iron atoms, with a minor relaxation of the total magnetic moment. Our results indicate that the carbon nanotube is slightly spin polarized and ferromagnetically coupled to the Fe aggregate.


Ali Moghaddam

Spin-dependent electron focusing in graphene

We show here that a ferromagnetic graphene can behave like an electron spin lens when its exchange energy becomes larger than the Fermi energy. The key property is that such a ferromagnetic (FM) graphene region exhibits a negative electronic refractive index for one spin direction and positive one for the other. As a result in a FM graphene sandwiched between two normal (N) regions, an unalloyed electronic beam in one left N side can be focused with a finite spin-polarization in the right N side. This produces a point spin accumulation with associated Friedel-like oscillations of the Fermi density of states. We propose that such a 2D concentration can be used as an electronic counterpart of the photonic chiral metamaterials, having a negative refractive index for only one direction of the circular polarization of photons.

Prasanta Kumar Muduli

Large local Hall effect in pin-hole dominated multigraphene

We report local and non-local measurements in pin-hole dominated micrometer-scale multigraphene spin-valves. Local spin-valve measurements show spurious switching behavior in resistance-voltage field sweeping similar to signal observed due spin injection to in multigraphene. The switching behavior has been explained in terms of local Hall effect at the pin-holes. Local-Hall effect appears due to large local fringe magnetic field produced at the pin-holes in AlOx tunnel barrier. The effect of local Hall effect is found to reduce as temperature is increased above 75 K. The strong local Hall effect in multigraphene although hinders spin injection into multigraphene has a lot of potential for device applications in its own.

Afdsh Namiranian

Effect of single magnetic impurities on spin-polarized transport of carbon nanotubes and graphene nanoribbons

Graphene and armchair single-wall nanotube, two nanostructure allotropes of carbon, are good quantum conductors. As it is known, in the ballistic regime the existence of a single impurity in a quantum conductor can make a noticeable effect on its conductance. Therefore, it is expected that the presence of a few number of single magnetic impurities can alter spin-polarized conductance of these systems as well.

We propose a general simple perturbative method to investigate the effect of single imperfection on the spin polarized transport of a quantum conductor lying between two spin-polarized electronics resistors. This method is employed for an armchair single wall carbon nanotube and a Gaphene nanoribbon, at the presence of single magnetic impurities, and the results show the spin polarized conductance is sensitive to the positions of impurities, geometry of carbon nanostructures and also relative spin orientations of electrons on the electrodes. Such dependence may be applicable if we remind that pushing the graphene may induce local magnetic moments on its surface.


Christoph Ohm

Readout of CNT vibrations using spin-phonon coupling

We theoretically study a double quantum dot consisting of a carbon nanotube with a suspended and a non-suspended part. We propose a scheme for spin-based detection of the nanotube bending motion in which the high vibrational frequency is down-converted to a lower, more accessible energy scale. We make use of the curvature-induced spin-orbit coupling in the carbon nanotubes [1,2,3]; in particular, in the presence of vibrations, this yields a weak effective spin-phonon coupling. Classical vibrations of the carbon nanotube are shown to induce a time-dependent magnetic field acting on the electrons confined to the suspended dot, thereby generating spin flips. Within a rotating-wave approximation we find that the weakness of the spin-phonon coupling results in an effective down-mixing of the high vibrational frequency of interest to a much lower spin-flip frequency and that the latter can be controlled by the strength of an externally applied magnetic field. We propose to read out the vibration-induced spin flips by measuring the leakage current through the double dot tuned to the Pauli-blockade regime as a function of the external magnetic field. From a master equation we predict that the leakage current shows a pronounced peak. The position of this peak allows for a read-out of the vibrational frequency.


Petr Ostrizek

Spin transport in graphene nanostuctures

Marek Rataj

Nonuniform Rashba coupling across a p-n junction in graphene

Niklas Rohling

Universal Quantum Computing with Spin and Valley Qubits

Universal two-qubit gates for spin qubits can be performed via Heisenberg-exchange interaction and local gates [1]. In graphene and carbon nanotubes the situation is changed by valley degeneracy as the tunneling between quantum dots couples spins as well as valleys. Considering each spin and each valley in two single-electron quantum dots as one qubit, unitary operations act on a space of 16 possible states. In this logic space we investigate quantum gates generated by exchange interaction and single-qubit operations.


Georgeta Salvan

Magne-Magnetic Study of Different Metal-Phthalocyanines by Combining Spectroscopic MOKE and Ellipsometry

Authors: Michael Fronk, Dietrich R.T. Zahn, Georgeta Salvan

In the past years organic materials experience much attention because of their potential application in spintronics devices due to their long spin life-times. This work focusses on the magnetoelectrical characterisation of paramagnetic phthalocyanines. While a part of this investigation (mainly on VOPc and CuPc) is already published [1], additional magneto-optical Kerr effect (MOKE) spectra of MnPc, FePc and CoPc will be presented. The magnetoelectrical Voigt constant is obtained from model calculations. A fit of the Voigt data using an oscillator model was performed in order to gain more insight in the electronic origin of the features in the Voigt constant and subsequently in MOKE. E.g. the hybridisation of Co-3d states to the HOMO-orbital of CoPc leads to additional features in the magnetoelectrical spectra compared to for example CoPc. This effect is much more pronounced in the magnetooptical spectra than in the dielectric function components that can be commonly accessed by spectroscopic ellipsometry.


Ralph Scheicher

Graphene Nano-Electrodes for DNA Sequencing

The proposal was made [1] that a graphene nanoganop could be used to probe the transverse conductance of individual nucleotides in DNA to rapidly identify the associated base sequence. This idea is innovative because atomically-thin electrodes made from graphene could overcome the difficult issue of achieving single-base resolution. Using first-principles methods, we evaluated different aspects of the performance of two graphene nano-electrodes configurations for base identification. In the first study [2], we investigated the electronic transport properties of the four nucleotides incorporated in the DNA current variation at finite bias due to changes in the nucleotides orientation and lateral position. Our second study [3] utilized molecular dynamics simulations in conjunction with electronic transport calculations to explore specifically the effect of the hydrogenated graphene edges on

Zhen-Gang Zhu
Magdalena Wojtaszek
Chi Vo Van
Cormac Toher
Sergio Tatay Aguilar

Maria Soriano
Manganese Phthalocyanine on Metallic Surfaces: From Kondo Effect to Magnetoresistance.

Understanding and controlling the magnetic moment of a molecule, in particular regarding its interaction with a substrate is a key issue in the emerging field of molecular spintronics. Transition metal phthalocyanines are particularly attractive since their magnetic properties are mostly determined by their active metal core, its interaction with the ligand field and the environment. Depending on the nature and concomitant coupling to the surface, the magnetic core can be manifested in a scanning tunneling spectroscopy (STS) in a variety of ways namely, i) zero-bias Kondo features, ii) inelastic electron tunneling spectroscopy signatures, or iii) magnetoresistance when using magnetic tips. Here, in collaboration with different experimental groups, we present studies of the manganese phthalocyanine (MnPc) deposited on different surfaces: Bi, Pb and Mn.

The magnetic core of the MnPc has three unpaired electrons. The adsorption on metal surfaces does not seem to change the magnetic moment of these molecules and an exciton Kondo effect arises due to the high magnetic moment. In order to understand the origin of this Kondo effect and to lay the foundations of a solvable Kondo model, we have carried out density functional theory calculations of the MnPc adsorbed on Bi and Pb. In addition, it has been shown that the adsorption of small molecules on the MnPc, such as carbon monoxide (CO), increases the Kondo temperature when deposited on Bi. Our calculations reveal that the number of unpaired electrons is reduced to one due to the change in the ligand field of the metal core. This reduction of the magnetic moment is compatible with the increased Kondo temperature, but the orbital hosting the unpaired spin is not concluding that the ligand of the metal core has to be taken into account to explain the Kondo effect of this system.

We also present our results of the MnPc adsorbed on Mn. Spin polarized STM/STS reveals magnetic contrast on these molecules when deposited on surfaces of different magnetic orientations. The contrast arises because the parallel and antiparallel currents are typically different. Using our package ALACANT (http://alacant.dft.ua.es), we have studied the magnetoresistance of the MnPc adsorbed on a Mn surface, i.e. the nature of the spin polarized current through an organic molecule, and the origin of the magnetic contrast in this system.

Karol Szalowski
Charge carrier-mediated interaction of impurity spins in triangular graphene nanoflakes

In the paper we present the results of tight binding approximation based calculations of Ruderman-Kittel-Kasuya-Yosida (RKKY) coupling between on-site and plaquette magnetic impurities in graphene nanoflakes. We take into account the coulombic interactions, which are of particular importance for RKKY interactions in graphene [3,4], by means of a Hubbard term. The interest is focused especially on the triangular nanoflakes, which are reported to exhibit interesting electronic structure [5]. We concentrate on the influence of charge carrier doping of the nanoflakes on the RKKY coupling sign and magnitude, with a view to identifying the conditions for robust ferromagnetic and antiferromagnetic interaction. Moreover, we study the magnetization distribution induced by the magnetic impurities (an analogue to Friedel oscillations) in the nanoflakes.

We investigated the model for the former case by means of a slave-boson method and introduce a symmetry. For that I develop a RF plasma technique to hydrogenate graphene in a controllable and reversible way. The alternative approach would be to verify these magnetic interactions in magnetoresistance measurements of defected graphene.

Sergio Tatay Aguilar
Nanodevices for spintronics with organic materials

Opto-electronically active magnetic molecules on metallic surfaces

Optoelectronically active organic molecules offer several advantages over traditional solid-state semiconductor materials in the fabrication of solar cells, including their low-cost, low weight, and flexibility. Here we present the results of ab initio density functional theory (DFT) and transport studies of molecules which combine two body dye molecule cores with a central metal atom to produce a molecule which is both magnetic and optoelectronically active. Two different central metal atoms are used for comparison: a Zn atom which DFT calculations indicate produces a non-magnetic molecule; and a Co atom which produces a magnetic molecule. These molecules were deposited on a metallic surface for study using a scanning tunneling microscope (STM). DFT calculations indicate that the magnetic molecule with the central Co atom should maintain its spin polarization on the substrate, and the STM dI/dV spectrum also shows evidence of spin effects.

Chi Vo Van
Magnetic properties of nanosized Co clusters on graphene on iridium

The structure and magnetic properties of Co clusters, comprising from 26 to 270 atoms, self-organized or not on the graphene(111) monolayer, were studied in situ with the help of scanning tunneling microscopy and X-ray magnetic circular dichroism. We evidence that the small clusters have almost no magnetic anisotropy and readily get damaged by soft X-rays. We find indication for a magnetic coupling between the clusters.

Magdalena Wojtaszek
Inducing magnetic interactions in graphene by hydrogen defects

Magnetism of carbon-based materials, containing only s and p electrons, as a counterpart of ferromagnetism in f-orbital metals (Fe, Co etc.), is of theoretical and technological interest. It is often explained by the alternation between sp2 orbitals and undercoordinated C-orbitals of sp3 hybridisation, occurring due to impurities, boundaries or defects [1]. These defects localize magnetic moments and lead to polarization of its electronic environment. Attempts to study this effect with FMF or SQPUD techniques in graphite were poorly reproducible, leaving the open question of the true origin of the ferromagnetic signal [2]. An alternative approach would be to verify these magnetic interactions in magnetoresistance measurements of defected graphene electronic device. For that I develop a RF plasma technique to hydrogenate graphene in a controllable and reversible way. The introduced defects are characterized by the ratio of the D and G band in Raman spectrum, what also allows us to determine the defect concentration. I will present systematic studies of electronic transport in graphene depending on plasma exposure time and report the influence of the amount of defects on graphene carrier mobilities and mean free path [3]. I will discuss the main scenarios leading to anomalous Hall Effect and signatures of intrinsic magnetization in such detected samples.

Zhen-Gang Zhu
Magnetic adatoms on graphene out and in the Kondo regime: an Anderson model treatment

We study theoretically the physical properties of a magnetic adatom on graphene out and in the Kondo regime based on an Anderson model. The specific model depends on the positions of the adatom. When it resides on one carbon atom, we infer an one-channel, two-flavor behavior. As it is located on the center of the honeycomb, we found a multichannel, multiflavor model by the symmetry.

We investigated the model for the former case by means of a slave-boson method and introduce a topological picture consisting of a degree of a map and a winding number (WN) to analyze the phase shift and the occupation on the impurity. The occupation is linked to the WN. For a generic normal metal we find a fractional WN. In contrast, the winding is accelerated by the relativistic dispersion of graphene at half-filling, in which case an integer occupation is realized. We show that the renormalization that shifts the impurity level is insufficient to invert the imdyarity level from below to above the Fermi energy. Consequently, the state at zero field is stable unless a gate voltage is tuned such that the Fermi energy touches the edge of the broadened impurity level. Only in this case is the zero field susceptibility finite and shows a pronounced peak structure when scanning the gate voltage. To study the properties of the magnetic adatom in the Kondo regime, we calculated analytically the selfenergies and the Green's function of the impurity

Doi: 10.1002/adfm.201002530

in presence of strong correlations. We find that the Kondo effect takes place only in a certain
energy range for the impurity level and while a gate voltage being applied to the graphene sheet.
This finding is in contrast to the Kondo resonance in a normal metal that may build up when
lowering the temperature. The origin of this behavior is traced back to the inherent properties
of graphene, especially its linear dispersion. The singularity in the full Green’s function
is also analyzed with the help of a transparent geometrical method, i.e. a singular ring in
a complex plane. It clearly identifies the conditions for presence of the Kondo resonance
or the singularity. The relations between the various selfenergies and the implications for
the experimental observations are discussed.