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Participant	Title	Abstract
Pier Paolo Baruselli	From density functional to Kondo: magnetic impurities on nanotubes	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 lineshapes to be expected are presently unknown. We explore this problem at the first principles atomistic 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 predicted Kondo temperatures and 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 foreshadow an interesting field and temperature dependence conductance, to be addressed in future experiments.
Sandip Bhattacharya	Microscopic approach to understanding the phase diagram and transport properties of pi-conjugated polymers	The field of organic spintronics has grown by leaps and bounds over the last few years because of the potential of organic semiconductors to match or even perform better than their inorganic counterparts in spintronic applications. It is now conceivable for organic materials to open new avenues to cheap, low-weight, mechanically flexible, chemically inert and bottom-up fabricated spin-devices. Furthermore the mechanisms responsible for the interaction of spins with their environment during transport are minimal for organic materials. This present work aims at providing insights into the challenging problem of charge and spin transport through organic semiconductors using fundamental microscopic models. We will outline a Monte Carlo study [1] of the finite temperature properties of a Hubbard-Peierls model describing pi-conjugated polymers. The model also incorporates spin-orbit coupling and hyperfine interactions and it is solved at the mean field level for half filling. In particular we explore the model as a function of the strength of electron-electron and electron-phonon interactions. At low temperature the system presents a non-spin-polarized to spin-polarized transition of local moments as the electron-electron interaction strength increases. At the same time by increasing the electron-phonon coupling there is a transition from a homogeneous to a Peierls dimerized geometry. As expected such a Peierls dimerized phase disappears at finite temperature due to thermal vibrations. More intriguing is the interplay between the electron-phonon and the electron-electron interactions at finite temperature. In particular we demonstrate that for a certain region of the parameter space there is a spin-crossover, where the system transits between its spin-states as the temperature increases. In close analogy to standard spin-crossover in di-valent magnetic molecules such a transition is entropy driven. Furthermore, we find that the phase diagrams are unaffected by hyperfine and spin-orbit coupling terms, as their coupling strengths are weak for organic polymers. Finally, we elaborate upon our transport set-up which consists, a network of polymer molecules described by the Hubbard-Peierls model sandwiched between two metallic leads. We measure the low-biased spin-polarized conductance using a Greens function approach [4] and the carrier mobility using linear response Kubo formalism. From these parameters we are able to extract useful quantities that characterize spin and charge transport, described by our microscopic theory. This part of the work, aims at understanding which out of hyperfine interaction or spin-orbit coupling is the more dominant contributor to spin scattering which would inhibit an efficient spin transport through organic polymers. We are also are interested in explaining the charge transport across model in different regimes of el-ph interaction strength and temperatures, with the model parameters extracted from first-principle constrained DFT calculations. [1] S. Bhattacharya, M.S. Ferreira and S. Sanvito, arXiv: 1012.3694, (2011). [2] S.Sanvito, Chem. Soc. Rev, 40, 3336-3355, (2011). [3] G. Szulczewski, S. Sanvito and M. Coey, Nat. Mat. 8, 693-695, (2010). [4] I. Rungger and S.Sanvito, Phys Rev B 78, 035407, (2008).
Lapo Bogani	Coupling molecular magnetic clusters and graphene into hybrids	
Thomas Brumme	Organometallic spin lattices	The formation of a well-ordered organometallic sheet consisting of two-dimensional polymeric phthalocyanine (polyFePc) was recently reported by Abel et al.[1]. The growth was also demonstrated on an insulating sodium chloride film which decouples the polyFePc from the metal substrate and thus leads to a preservation of the intrinsic properties of the polymeric film. In this work we investigate theoretically the electronic and magnetic properties of a single layer of polyFePc by means of DFT and DFT+U calculations. DFT calculations suggest an antiferromagnetic ground-state which is at least 57 meV lower in energy than the ferromagnetic state, whereas the ferromagnetic arrangement is preferred within DFT+U - by at least 250 meV. This observation suggests that the polyFePc system represents a square-lattice arrangement of molecular spins which is stable at room temperature. Furthermore, we discuss the influence of different substrates on the electronic properties and the transport characteristics of the polyFePc system. [1] M. Abel, S. Clair, O. Ourdjini, M. Mossoyan, and L. Porte, JACS 133, 1203 (2011)
Jan Bundesmann	Electron transport and spin in graphene	The weak atomic spin-orbit interaction (SOI) in graphene leads to the assumption of large spin relaxation times. Simulations, taking into account spin-scattering from charged impurities in the substrate, yielded spin relaxation times [1] much larger than spin injection experiments in graphene[2,3]. Still assuming that the model of spins scattered at charged impurities is correct, we implemented a tight-binding model for graphene in the presence of SOI. In our work the focus lies on the effects of SOI on electron transport (i.e. low energy excitations and the role of symmetry classes manifested, e.g., in weak localization) as well as its influence on spin transport in the diffusive regime. References [1] Ertler, Konschuh, Gmitra and Fabian, Phys. Rev. B 80, 041405(R) (2009) [2] Tombros, Josza, Popinciuc, Jonkman and van Wees, Nature 448, 571 (2007) [3] Han, Pi, McCreary, Li, Wong, Swartz and Kawakami, Phys. Rev. Lett. 105, 167202 (2010)
Alessandro Cresti	Electronic transport in epoxide and methyl functionalized graphene nanoribbons	
Miriam del Valle	Spin transport in carbon nanotubes in a parallel magnetic field with spin-orbit interaction	Reversible spin-polarized currents through finite-size carbon nanotubes can be obtained upon tuning a threading magnetic field, exploiting the curvature-induced spin-orbit splitting. We will analyze this phenomenon and thoroughly discuss the contribution of the different effects competing in the evolution of the transport characteristics in the magnetic field. Analytical results are supported by numerical simulations for different lengths and chiralities.
Ginetom Diniz	Electronic Transport in Carbon Nanotubes: Spin-Orbit Coupling Effects	In this work, we have investigated the role of spin-orbit coupling (SOC) on the conductance response of carbon nanotubes (CNT). We have analyzed different SOC mechanisms: Rashba spin-orbit Interaction (RSO), induced by an extrinsic source of electric field and Intrinsic Spin-Orbit interaction (ISO), originated from the symmetry properties of the honeycomb lattice. For the RSO, three different electric field directions was studied: (i) radial field, (ii) perpendicular field and (iii) helical field. For the helical field, we have obtained a very remarkable result: a non-zero current of polarization due to the chiral symmetry of the field. Our results may be suitable for further application of CNT's in the spintronic field, using SOC to effectively control the spin-polarized transport in eletronic devices as well as molecule detectors by exploring the nature of SOC.
Andrea Donarini	Interference effects in the Coulomb blockade regime: Current blocking and spin preparation in symmetric nanojunctions	
Simone Fratini	Spin relaxation in organic molecules	
Rico Friedrich	Determining the decisive spin states for the optical absorption behavior of manganese phthalocyanine by density functional theory	For the fabrication of molecular spintronics devices a detailed understanding of the electronic structure of the used systems will play a key role. Therefore spectroscopic investigations as for example optical absorption measurements are very important since they offer direct insight into the electronic states of the molecule. Here we show experimental and theoretical results for manganese phthalocyanine whose optical absorption behavior is quite special among other metal phthalocyanines. We point out that this might be attributed to the formation of charged species during the excitation process. Then the spectra are determined by a spin ordering of the spectral signals.

Bo Gao	Gate controlled linear magneto-resistance in thin Bi2Se3 films	We report magnetotransport data gained from thin Bi2Se3 films under the action of a backgate voltage. Upon application of high negative gate voltages, the sheets display linear magnetoresistance (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 magnetoresistance model that includes a linear B-field dependence of the surface 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 Abrikosov's quantum magnetoresistance 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. [1]. Abrikosov, A. A. Quantum magnetoresistance Phys. Rev. B. 58, 2788-2794 (1998)
Benjamin Göhler	Spin Selectivity in Electron Transmission Through Self-Assembled 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 vapours 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 10E-4 [1]. Here we present a similar experiment where electrons emitted from a gold surface and transmitted through a monolayer of self assembled double stranded DNA molecules are highly spin-polarized. Since photoelectrons excited with linearly polarized light from a gold surface are not spin polarized, the chiral DNA molecules act as very efficient spin filters achieving a spin polarization of up to 60% [2]. To measure the spin polarization a compact Mott polarimeter has been constructed and calibrated (effective Sherman function: Seff = -22,9%). Laser radiation of 213nm (5.8eV) is chosen to excite the photoelectrons. This photon energy is sufficient to emit photoelectrons out of the gold substrate, but not to ionize the molecules. The spin selectivity is observed at room temperature and extremely high as compared with other known spin filters. A systematic study shows that the spin filtration efficiency depends on the length of the DNA molecules adsorbed on the gold surface and its organization. [1] S. Mayer, J. Kessler, Phys. Rev. Lett. 74, 4803 (1995). [2] B. Göhler et. al, Science, 331, 894 (2011)
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 Rashbalike 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 charges in the system and allows even weak 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. In this talk, we will show that in spintronic setups involving states with spin > 1/2 the spin-quadrupole moment has to be treated as a additional 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 simplest relevant 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 an 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 various new 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] (coupling to the quantum dot spin-dipole moment), which was demonstrated to be electrically tuneable in a carbon-nanotube spin-valve [4]. However, we find that there is an additional quadrupolar exchange field that couples to the spin-quadrupole moment thereby influencing the spin-dipole and charge accumulations in a new way: it gives 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. [1] M. Baumgärtel, M. Hell, S. Das, M. R. Wegewijs, arXiv:1009.5874 [2] B. Sothmann and J. König, Phys. Rev. B 82, 245319 (2010) [3] J. König and J. Martinek, Phys. Rev. Lett. 90, 166602 (2003). [4] J. R. Hauptmann, J. Paaske, and P. E. Lindelof, Nat. Phys 4, 373 (2008).
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-dimensional correlated electrons with uniform, Rashba plus Dresselhaus, spin-orbit coupling. For different values of the wave number of the modulation, commensurate with different diameters of the, characterized by four Fermi point Fermi surface of the system, we shown 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 field theory approach, 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.
Alan 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 sign as the applied gate voltage changes. We have demonstrated [2] that these anomalies arise from “universal” mesoscopic resistance 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. [1] A.B. Kaiser and V. Skakalova, Chem. Soc. Rev. 40, 3786 (2011). [2] V. Skakalova, A.B. Kaiser, J.S. Yoo, D. Obergfell. and S. Roth, Phys. Rev. B 80, 153404 (2009). [3] H.J. Park, V. Skakalova, C.W. Bumby, D.S. Lee, T. Iwasaki, J. Meyer, U. Kaiser and S. Roth, Phys. Stat. Sol. B 247, 2915 (2010). [4] A.B. Kaiser, C. Gomez-Navarro, R.S. Sundaram, M. Burghard and K. Kern, Nano Letters 7, 1787 (2009). [5] S. Ravi, A.B. Kaiser and C.W. Bumby, Chem. Phys. Lett. 496, 80 (2010).
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 edge 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 and the presence of edge defects further destabilize the intrinsic magnetism of such systems. We conclude that edge magnetism within graphenes 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 [1] J. Kunstmann, C. Ozdogan , A. Quandt, H. Fehske, Phys. Rev. B 83, 045414 (2011).
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.
Lakhaphat Lin Aigu	89% Positive Magnetoresistance in PANI-NP nanocomposites at Room Temperature	We demonstrate a polyaniline-iron oxide nanoparticle (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 isomer of the cluster 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 structural 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 is not found 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 reduction of the total magnetic moment. Our results indicate that the carbon nanotube is slightly spin polarized and ferromagnetically coupled to the Fe aggregate. [1] Mañanes A., Duque F., Ayuela A., López M. J., Alonso J. A., Phys. Rev. B, 78, 35432 (2008)
Ali Moghaddam	Spin-dependent electron focusing in graphene	We show here that a ferromagnetic graphene can behave like a electronic 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 unpolarized 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 local spin density. Our study also reveals that FM graphene can behave like a 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 spin-valves.	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 during field sweeping similar to signal observed due spin-injection in to 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.
Afshin 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 small imperfectness on the spin polarized transport of a quantum conductor lying between two-spin polarized electron reservoirs. This method is employed for an armchair single wall carbon nanotube and a Garphene 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. [1] T. Ando, J. Phys. Soc. Jpn. 69, 1757 (2000); Kuemmeth et al., Nature 452, 448 (2008); Jespersen et al. Nat. Phys. 7, 248 (2011). [2] K. Flensberg and C. M. Marcus, Phys. Rev. B, 81, 195418, (2010). [3] A. Pályi and G. Burkard. Phys. Rev. Lett. 106, 086801 (2011).
Petr Ostrizek	Spin transport in graphene nanostructures	
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. [1] D. Loss and D. P. DiVincenzo, Phys. Rev. A 57, 120 (1998)
Georgeta Salvan	Magneto-Optical 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 spintronic devices due to their long spin life-times. This work focusses on the magnetooptical 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 magnetooptical Voigt constant is obtained using optical 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 magnetooptical spectra compared to for example CuPc. This effect is much more pronounced in the magnetooptical spectra than in the dielectric function components that can be commonly accessed by spectroscopic ellipsometry. [1] M. Fronk et al., Phys. Rev. B 79 (2009) 235305
Ralph Scheicher	Graphene Nano-Electrodes for DNA Sequencing	The proposal was made [1] that a graphene nanogap 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 when located in a graphene nanogap. In particular, we determined the electrical 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

		the translocating DNA. It is found that these edge-hydrogenated graphene electrodes can facilitate the temporary formation of H-bonds with suitable atomic sites in the nucleotides, leading to drastically increased conductivity and significantly reduced statistical variance. [1] “Rapid Sequencing of Individual DNA Molecules in Graphene Nanogaps”, H. W. Ch. Postma, Nano Lett. 10, 420 (2010). [2] “Transverse Conductance of DNA Nucleotides in a Graphene Nanogap from First Principles”, J. Prasongkit, A. Grigoriev, B. Pathak, R. Ahuja, and R. H. Scheicher, Nano Lett. 11, 1941 (2011). [3] “Enhanced DNA Sequencing Performance Through Edge-Hydrogenation of Graphene Electrodes”, Y. He, R. H. Scheicher, A. Grigoriev, R. Ahuja, S. Long, Z. L. Huo, and M. Liu, Adv. Funct. Mater., published on-line May 9, DOI:10.1002/adfm.201002530
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 and its interaction with the ligand field and the enviroment. Depending on the nature and concomitant coupling to the surface, the magnetic core can be manifest in 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 exotic 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 adsorpted 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.dfa.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	Magnetism of graphene nanostructures has recently focused increasing attention [1]. The graphene nanoflakes constitute promising building blocks of the future spintronics devices (e.g. [2]). This provides a sound motivation for studies of magnetic properties emerging in small graphene structures. 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. [1] O. V. Yazyev, Rep. Progr. Phys. 73, 056501 (2010) [2] M. Ezawa, New J. Phys. 11, 095005 (2009) [3] A. M. Black-Schaffer, Phys. Rev. B 81, 205416 (2010) [4] K. Szaowski, arXiv:1106.4233v1 (2011) [5] M. Ezawa, arXiv:1101.3612v1 (2011)
Sergio Tatay Aguilar	Nanodevices for spintronics with organic materials	
Cormac Toher	Opto-electronically active magnetic molecules on metallic surfaces	Opto-electronically 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 bodipy dye molecule cores with a central metal atom to produce a molecule which is both magnetic and opto-electronically 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 2700 atoms, self- organized or not on the graphene/Ir(111) moiré, 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 d, 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 MFM or SQUID 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 defected samples. [1] O. V. Yazyev and L. Helm, Phys. Rev. B, 75, 125408 (2007) [2] P. Esquinazi, et al., J. Magn. Magn. Mater. (2009) [3] M. Wojtaszek et al. submitted to J. Appl. Phys.
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 impurity level from below to above the Fermi energy. Consequently, the state at half-filling 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

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.