TT 7: Spintronics I (joint session DS, HL, MA, TT, organized by HL)

Time: Monday 9:30–13:00 Location: POT 151

TT 7.1 Mon 9:30 POT 151

Dynamical spin-orbit-based spin transistor — •Fahriye Nur Gürsoy[1,2], Phillipp Reck[1], Cosimo Gorini[1], Klaus Richter[1], and Inanç Adagideli[2] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Faculty of Engineering and Natural Sciences, Sabanci University, Orhanli-Tuzla, Istanbul, Turkey

Spin-based devices are highly important for the future of information technology. In this project we focus on a mesoscopic 2-Dimensional Electron Gas (2DEG) with time-dependent Rashba spin-orbit interaction, which can be engineered via an AC top gate.

Spin-orbit coupling in 2DEGs can be rewritten in terms of appropriate SU(2) gauge fields, so as to clearly identify the relevant Onsager symmetries [1, 2].The latter can then be exploited for the realisation of spin transistor devices, in particular when the spin-orbit interaction is non-homogeneous through the sample [1]. On the other hand, a dynamical Rashba interaction was suggested as a generator of spin-motive forces. Here we merge the two concepts, and explore the possibilities of realising a spin transistor in a quantum coherent sample driven by a time-dependent Rashba field. We follow a mixed analytical-numerical approach, and compute the (spin) conductance and the pumping (spin) current of the periodically driven system with the Floquet Hamiltonian method [3].

[1] I. Adagideli, et al., Phys. Rev. Lett. 108, 236601 (2012).
[2] C. Gorini, et al., Phys. Rev. Lett. 109, 246604 (2012).
[3] J. H. Shirley, Phys. Rev. 138, B979 (1965).

TT 7.2 Mon 9:45 POT 151

Coherent electron Zitterbewegung triggered by ps optical pulses — •Manfred Ersfeld[1], Ivan Stepanov[1], Alexander V. Poshakinskiy[2], Mihail Lepsa[3], Eugeneous L. Ivchenko[2], Sergey A. Tarasenko[2], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany — [2]Ioffe Institute, 194021 St Petersburg, Russia — [3]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH, Germany

Zitterbewegung is a direct consequence of relativistic quantum mechanics which predicts that free Dirac electrons exhibit a rapid trembling motion even in the absence of external forces. Recent theoretical studies have shown that electrons in III-V semiconductors also exhibit Zitterbewegung caused by the spin orbit interaction. Here we probe the Zitterbewegung of electrons in n-type InGaAs as an AC electric current. We trigger the coherent electron Zitterbewegung by optical initialization of an ensemble of electron spins in the same spin states and control the frequency of electron oscillations in real space by tuning the Larmor spin precession frequency in an external magnetic field.

TT 7.3 Mon 10:00 POT 151

On the link between charge- and spin-dynamics in PBTTT — •Uday Chopra[1], Erik R. McNellis[1], Denis Andrienko[2], Pascal Kordt[2], and Jairo Sinova[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

In the nascent field of organic spintronics, charge- and spin-dynamics are strongly linked. We study this relationship in a high-mobility[1], spin-conducting polymer[2], PBTTT, using a newly developed multi-scale modelling framework. High mobility ($\sim 1\ cm^2V^{-1}s^{-1}$) in PBTTT along the $\pi-\pi$ stacking direction is attributed to its highly ordered structure and hence the strong transfer integrals in the same direction. However, the mechanism for spin transport and its correlation with electron transport is still unclear. We demonstrate the anisotropy in electron dynamics of PBTTT by calculating electron transfer rates for morphologies of different sizes and extent of disorder in the backbone using Marcus theory and Kinetic Monte Carlo (KMC) as implemented in VOTCA-CTP[3] and showing the field and temperature dependence of mobility along different crystalline axes. In addition to it, we present an approach for spin transport in organic semiconductors build on top of VOTCA-CTP via first-principles modelling of spin relaxation mechanisms which allows us an uprecedented insight into the explicit dependence of spin- on charge-dynamics and the parameters that correlate them. [1] McCulloch et al., Nat. Mater., 2006, 5, 328. [2] Watanabe et al., Nat. Phys., 2014, 10, 308. [3] V. Rühle et al. J Chem. Theory Comput., 2011, 7, 3335.

TT 7.4 Mon 10:15 POT 151

Theory of current-induced spin polarisations in a 2DEG — Amin Maleki[1], •Cosimo Gorini[2], Ka Shen[3], Ilya V. Tokatly[4,5], Giovanni Vignale[6], and Roberto Raimondi[1] — [1]CNISM e Dipartimento di Fisica, Università Roma Tre, Rome, Italy — [2]Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany — [3]Kavli Institute of NanoScience, Delft University of Technology, Delft, Netherlands — [4]Nano-Bio Spectroscopy group, Dpto. Fisica de Materiales, Universidad del País Vasco, San Sebastián, Spain — [5]IKERBASQUE, Bilbao, Spain — [6]Department of Physics and Astronomy, University of Missouri, Columbia, Missouri, USA

The Bloch equations for the spin dynamics of a 2DEG are derived in the presence of intrinsic (Rashba and Dresselhaus) and extrinsic (impurities) spin-orbit coupling. In comparison to previous analyses, we find new terms arising from the interplay between the two types of spin-orbit interaction. These influence current-induced spin polarisations (CISP), which are shown to have a more complex symmetry with respect to that of the internal Rashba-Dresselhaus field. Our results are derived both diagrammatically and via a semi/quasi-classical approach, based on a SU(2) gauge formulation of spin-orbit coupling.

TT 7.5 Mon 10:30 POT 151

Toward accurate calculation of diffusive spin transport starting from realistic Hamiltonians. Applications to electrons, excitons, and topological insulators. — •Vincent Sacksteder[1] and Yasufumi Araki[2] — [1]W155 Wilson Building, Royal Holloway University of London, Egham Hill, Egham, TW20 0EX, United Kingdom — [2]Creative Interdisciplinary Research Division, Tohoku University

Spin-orbit couplings, in the presence of an electric current, can generate strong spin currents with possible applications to magnetic domain switching in new memory devices. This talk will focus on a coarse-graining strategy which starts from realistic Hamiltonians describing spin and scattering at the atomic scale, and derives spin diffusion equations suitable for modeling a spintronics device. After reviewing the standard formalism, we outline how spin diffusion coefficients can be calculated either analytically or numerically, in either magnetized or unmagnetized systems. We present results for spin lifetimes, spin polarization production, and characteristic spatial patterns in electron gases, excitons, and topological insulators.

TT 7.6 Mon 10:45 POT 151

Charge- and Spin Dynamics in Organic Spintronics from First-Principles Theory: VOTCA-STP — •Erik R. McNellis[1], Shayan Hemmatiyan[1,2], Amaury Melo Souza[1], Sebastian Müller[1], Sergei A. Egorov[1,3], Denis Andrienko[4], and Jairo Sinova[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Texas A & M University, College Station, USA — [3]University of Virginia, Charlottesville, USA — [4]Max-Planck-Institute for Polymer Research, Mainz, Germany

Novel high-mobility materials based on organic molecules bring a host of advantages in spintronic applications. In organics, spin- and charge dynamics are intimately linked. Ideally, such materials should be theoretically modeled using realistic structural models with atomic resolution, and field- and spin-orbit coupling (SOC) effects calculated from state-of-the-art first-principles theory.

We present a multi-scale framework for modeling of spin-dynamics in organics, implemented on top of the electron dynamics given by the VOTCA-CTP package[1]. This development allows us to accurately treat the balance of SOC phenomena in realistic morphologies, while observing the link between charge- and spin-dynamics directly.

Our results include a complete map of the spin-relaxation in Alq_3 - the organic spintronics fruit-fly - as a function of charge concentration and temperature. Additionally, insights into the highly spin conducting polymer PBTTT will be presented, along with developments towards treating the spin Hall and Nernst effects.

1. V. Rühle et al., J Chem. Theory Comput. **7**, 3335 (2011)

Coffee Break

TT 7.7 Mon 11:30 POT 151

Control of spin helix symmetry in semiconductor quantum wells by crystal orientation — •Paul Wenk, Michael Kammermeier, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We investigate the possibility of spin-preserving symmetries due to the interplay of Rashba and Dresselhaus spin-orbit coupling in n-doped zinc-blende semiconductor quantum wells of general crystal orientation. It is shown that a conserved spin operator can be realized if and only if at least two growth-direction Miller indices agree in modulus. We determine the appropriate requirements on the axial symmetric Rashba and Dresselhaus contributions and discuss the impact of cubic Dresselhaus terms which break this symmetry. We observe that including the latter commonly inhibits a perfect realization of the persistent spin helix symmetry except for two specific directions, i.e., [110] and [111]. Furthermore, by analyzing the spectrum of the spin diffusion equation, we show that besides the cases of perfect spin-preserving symmetries, the spin of the long-lived homogeneous spin state relaxes about a factor 2 faster than for the helical spin state. To support experimental probing, we additionally provide analytical expressions for the weak (anti)localization correction and the characteristic shift of the magnetoconductivity minima [2] which show an imprint of the peculiar symmetry.

[1] M. Kammermeier *et al.*, Phys. Rev. Lett. **117**, 236801 (2016)
[2] K. Yoshizumi *et al.*, Appl. Phys. Lett. **108**, 132402 (2016).

TT 7.8 Mon 11:45 POT 151

Hidden orbital polarization in centrosymmetric materials — •Ji Hoon Ryoo and Cheol-Hwan Park — Department of Physics & Astronomy, Seoul National University 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea

Until recently, the possibility of spatial spin distribution in centrosymmetric and non-magnetic materials was largely dismissed, because their electronic bands are degenerate even if spin-orbit coupling is strong. However, Zhang et al. [1] has pointed out that even in those materials, the degenerate Bloch states can have spin polarization localized at different sites in real space, significantly broadening the scope of spintronics to materials with inversion symmetry. On the other hand, the orbital magnetic moment could play as an important role as the spin moment in the magnetization of solids, in both equilibrium and non-equilibrium situations [2-5]. In this talk, we report that the hidden, or sublattice-dependent orbital polarization of Bloch states can be large in common centrosymmetric materials, and suggest some implications of this finding to photoemission spectroscopies and antiferromagnetic information technology.

1. X. Zhang et al., Nat. Phys. 10, 387 (2014).
2. R. A. Reck and D. L. Fry, Phys. Rev. 184, 492 (1969).
3. D. Ceresoli et al., Phys. Rev. B 81, 060409 (2010).
4. T. Yoda, T. Yokoyama, and S. Murakami, Sci. Rep. 5, 12024 (2015).
5. S. Zhong, J. E. Moore, and I. Souza, Phys. Rev. Lett. 116, 077201 (2016).

TT 7.9 Mon 12:00 POT 151

Improving and tailoring the magnetic properties of thin Fe layers by making use of exchange coupling — •Markus Ehlert, Helmut Körner, Thomas Hupfauer, Markus Schitko, Christian Back, Günther Bayreuther, and Dieter Weiss — Institute of Experimental and Applied Physics, University of Regensburg, Germany

The control of the magnetic properties of thin ferromagnetic films is crucial for the functionality of spintronic devices, e.g., for the detection of the spin Hall effect [1]. The goal of our work is to improve the magnetic stability of commonly used Fe layers by making use of the exchange coupling between soft magnetic Fe and hard magnetic Dysprosium (Dy). Microstructured thin films of Fe, Dy, and Fe-Dy multilayers were prepared by electron-beam lithography and ultra-high vacuum sputtering. The magnetic properties of the materials were determined by means of the AMR effect. By analyzing and comparing the corresponding AMR data we show that the presence of a Dy layer on top of the Fe layer significantly influences and enhances the magnetic properties of the Fe layer. We also investigated the temperature dependence of this effect and its dependence on the thickness of the Fe layer. All experimental results can consistently be explained with the model of the AMR effect and are also confirmed by corresponding SQUID measurements of full film samples.

[1] M. Ehlert *et al.*, Phys. Status Solidi B **251**, 1725-1735 (2014).

TT 7.10 Mon 12:15 POT 151

First principles calculations to address key spin relaxation mechanisms in organic semiconductors — •Amaury de Melo Souza[1], Sergei Ergorov[2], Pedro Brandimarte[3], Sebastian Mueller[1], Uday Chopra[1], Shayan Hemmatiyan[4], Denis Andrienko[5], Ilja Mueller[1], Jairo Sinova[1], and Erik McNellis[1] — [1]Johannez Gutenberg University, Mainz, Germany — [2]University of Virginia, Charlottesville, USA — [3]University del Pais Vasco, San Sebastian, Spain — [4]Texas A&M University, College Station, USA — [5]Max Planck Institute for Polymers, Mainz, Germany

In this work, we present our theoretical framework to simulate simultaneously spin and charge transport in amorphous organic semiconductors. By combining several techniques e.g. molecular dynamics, density functional theory and kinetic Monte Carlo, we are able to study spin transport in the presence of anisotropy, thermal effects, magnetic and electric field effects in realistic morphologies of amorphous organic systems. In this talk, we present in detail first-principles calculations combined with perturbation theory in order to extract the relevant quantities required to address key spin relaxation mechanisms, namely, spin flip due to spin-orbit coupling, intra-site spin relaxation due to spin-orbit coupling and electron-phonon coupling and exchange mediated transport. Finally, we apply our approach to a realistic morphology of Alq3 (Tris(8-hydroxyquinolinato)aluminum) and identify which spin relaxation mechanism is dominant in this system.

Invited Talk TT 7.11 Mon 12:30 POT 151

Carbon nanotubes as excitonic insulators — •Massimo Rontani — CNR-NANO, Modena, Italy

Fifty years ago Walter Kohn speculated that a zero-gap semiconductor might be unstable against the spontaneous generation of excitons—electron-hole pairs bound together by Coulomb attraction. The reconstructed ground state would then open a gap breaking the symmetry of the underlying lattice, a genuine consequence of electronic correlations.

I will show that this 'excitonic insulator' is realized in zero-gap carbon nanotubes, by presenting results of first-principles calculations performed by means of many-body perturbation theory as well as quantum Monte Carlo. The excitonic order modulates the charge between the two carbon sublattices of the armchair tube, opening an experimentally observable gap which scales as the inverse of the tube radius and weakly depends on the axial magnetic field.

These findings invalidate the common wisdom that the ground state of armchair carbon nanotubes is a Luttinger liquid. I will discuss the physical origin of this conclusion, related to the strong e-h binding in quasi-1D and the almost unscreened long-range interactions in undoped nanotubes. Finally, I will propose independent experimental tests to discriminate between the excitonic insulator and the Luttinger liquid at strong coupling (Mott insulator).

This work is performed together with Daniele Varsano, Sandro Sorella, Davide Sangalli, Matteo Barborini, Stefano Corni, and Elisa Molinari.