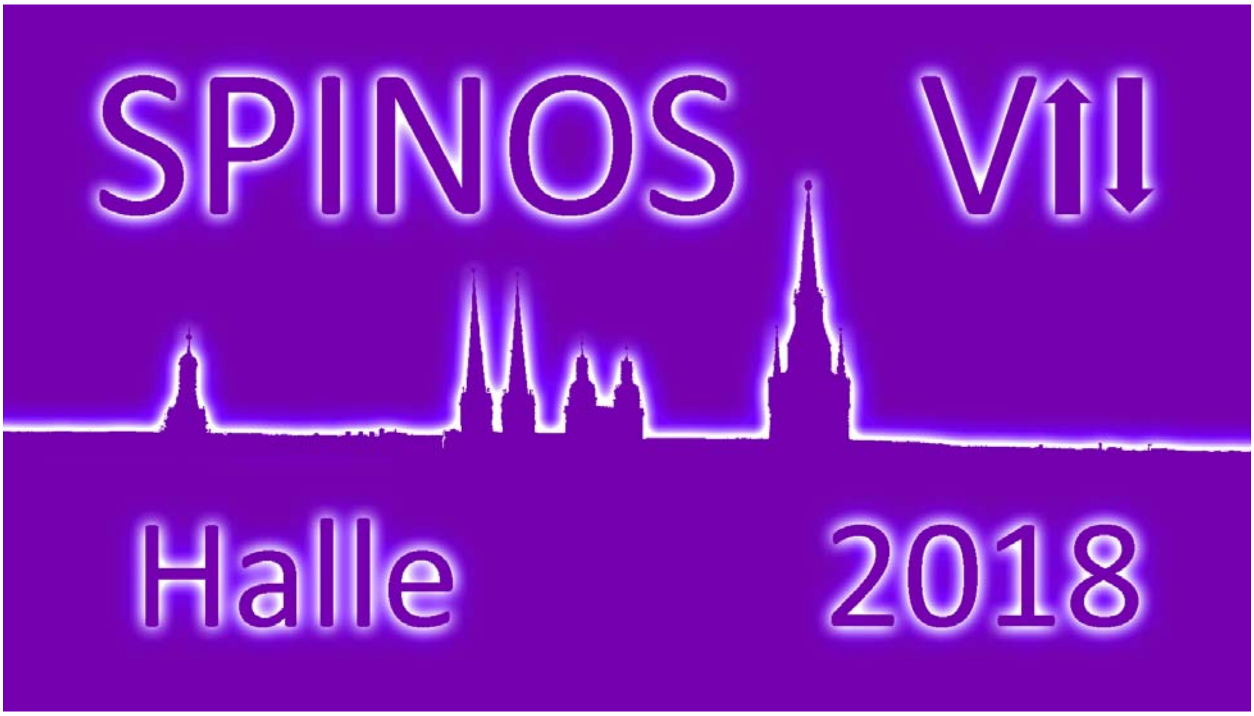
7th International Conference on Spins in Organic Semiconductors

August 13 - August 16, 2018
Halle (Saale), Germany



Book of Abstracts

MARTIN-LUTHER-UNIVERSITÄT
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Welcome

SPINOS, the International Meeting on Spins in Organic Semiconductors is the name of a series of conferences that started in 2007 in Bologna and continued successfully in Salt Lake City (2009), Amsterdam (2010), London (2012), Himeji (2014), and Chicago (2016). The goal of SPINOS is to bring together scientists investigating spins in organic semiconductors and carbon based systems and to discuss recent advances in organic spintronics, magnetic field effects in organic systems, organic magnets, and spin chemistry. Material systems of interest include p-conjugated polymers and small molecules, but also carbon based systems like Graphene. Besides the possibility to monitor the progress of established areas of organic spintronics the conference also tries to show up new directions and opportunities for spins in organic materials.

Goals

SPINOS is established as an international meeting to present and to discuss physics and applications in organic semiconductors. The meeting addresses spins in organic materials including semiconducting polymers and graphene. The effects discussed range from basic physics of spin pumping and spin polarized transport or molecules on magnetic interfaces (spinterfaces) to magnetoresistive effects and their device applications or the significance of electron spins in the development or organic LEDs. Also SPINOS is always open for new related areas.

This way SPINOS brings together researchers from different areas and different continents and presents a common meeting ground for four days.

Topics

- Organic spintronics
- New methods of generating spin currents, including spin Hall effects and spin pumping
- Magnetic field effects in organic materials
- Organic magnets
- Spin chemistry
- Spin statistics in organic semiconductor materials and devices and other spin-related phenomena in organic materials

Local organization

Prof. Georg Schmidt
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International advisory committee

K. Awaga	(Nagoya University, Japan)
D. Awschalom	(Universiy of Chicago, USA)
P. Bobbert	(Eindhoven University of Technology, The Netherlands)
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W. van der Wiel	(Twente University of Technology, The Netherlands)
M. Wohlgenannt	(University of Iowa, USA)
Z. Valy Vardeny	(University of Utah, USA)

Local conference information

Registration

Participants can register at the welcome reception in the Löwengebäude on Sunday evening. Later registration can be done at the conference site during the whole conference.

Lunch and coffe breaks

On Monday and Tuesday lunch will be provided at the conference site. Coffe breaks will also be on site on all days of the conference.

Posters

Posters should be put on the poster boards during the coffe break on Monday morning and can be taken down during the coffe break on Thursday morning. The poster room is located directly besides the room where coffe and lunch are served. So posters can be visited during all breaks. On Monday and Tuesday evening official poster sessions take place where poster presenters should be available for discussion.

Excursion

The excursion takes place on Wednesday afternoon and starts with a boat trip on the river Saale with the MS-Händel II at 4.30 pm. At 6 pm Buses will take the participants to the champagne making facility of Rotkäppchen (largest manufacturer of sparkling wine in Europe) in Freyburg where a guided tour through the fabrication and a short champagne tasting will take place.

Banquet

After the champagne tasting the conference Banquet will be held at the site of Rotkäppchen. After the Banquet at 11 pm busses will take the participants back to Halle.

Locations

Reception at the Aula

The welcome reception and registration will take place at the Aula (Auditorium) of Halle University in the so called Löwengebäude (Address: Universitätsplatz 11, 06108 Halle/Saale). An easy way to get there is by tram to the station ‚Moritzburgring'.
For example from:
Zentrum Neustadt (Tryp Hotel) Tram #2
Marktplatz or Hallmarkt (B&B Hotel) Tram #2 (also #1, #7, #8 from Marktplatz)
Riebeckplatz (Dorint) -> Moritzburgring : Linien 2 oder 7

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Conference location: Lepoldina

The conference will be held at the German Academy of Sciences Leopoldina (Address: Jägerberg 1, 06108 Halle/Saale).
An easy way to get there is by tram to the station ‚Moritzburgring‘.
For example from:
Zentrum Neustadt (Tryp Hotel) Tram #2
Marktplatz or Hallmarkt (B&B Hotel) Tram #2 (also #1, #7, #8 from Marktplatz)
Riebeckplatz (Dorint) -> Moritzburgring : Linien 2 oder 7

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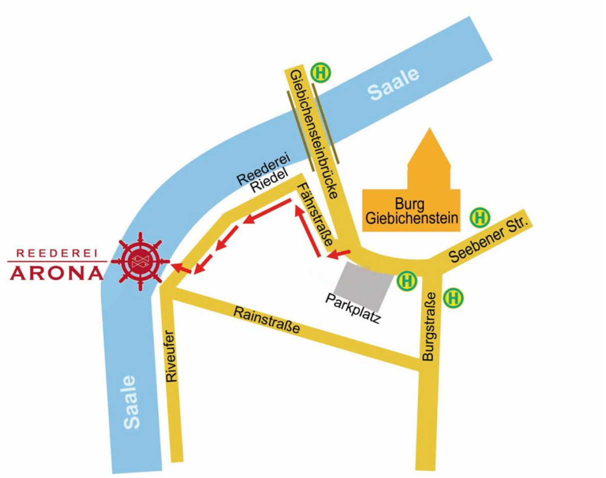
Excursion

The excursion on August 15 starts with a boat trip on the river Saale with the MS-Händel II.



People should be at the landing at 4.15 pm, the trip starts at 4.30 pm. At 6 pm we will be back and buses will bring us from the landing to the facilities of Rotkäppchen for a guided tour and the banquet. After the banquet the buses will bring us back to Halle.

Schedule

Sunday, August 12

18:00-21:00 Registration and welcome reception at the Aula/Löwengebäude

Monday, August 13

Session 1 (Session Chair: E. Coronado)

08:40-09:00 Opening remarks
G. Schmidt

09:00-09:30 I-1: „Signature of Exchange Bias and Room Temperature Magnetic Order in Molecular Layers“
M. Gruber

09:30-10:00 I-2: „Magnetic Subunits Within a Single Molecule-Surface Hybrid“
D. Bürgler

10:00-10:30 I-3: „How to Probe the Spin Contribution to Momentum Relaxation in Topological Insulators“
A. Ardavan

Coffee break

Session 2 (Session Chair: A. Ardavan)

10:50-11:10 O-1: „Hybrid Materials Featuring Molecular Quantum Bits“
J. van Slageren

11:10-11:30 O-2: „Nonlinear light-matter interaction: from superconducting qubits to spins in diamond“
E. Buks

11:30-11:50 O-3: „Resistive bistability in organic spintronic devices and applications to neuromorphic computing“
A. Riminucci

Lunch break at Leopoldina

Session 3 (Session Chair: Not yet confirmed)

12:50-13:20 I-4: „Direct evidence of spin injection in the HOMO/LUMO levels of a molecular material using a Spin-OLED device“
E. Coronado

13:20-13:40 O-4: „Abrupt Change of Ligand Fields During Formation of Molecular Contacts“
T. Balashov

13:40-14:00 O-5: „Nanoscale Studies of Organic Radicals: Surface, Interface, and Spinterface“
M. B. Casu

14:00-14:20 O-6: „Electric Field Mediated Coherent Spin Tuning in Antiferromagnetic Molecular Magnets“
J. Liu

Coffee break and posters

Session 4 (Session Chair: Not yet confirmed)

14:40-15:10 I-5: „Triplet interaction processes in phosphorescent and TADF-based OLEDs“
R. Coehoorn

15:10-15:30 O-7: „High Magnetic Field Effects in Organic Light Emitting Diodes“
E. Ehrenfreund

15:30-15:50 O-8: „Electrical Detection of Ferromagnetic Resonance with an Organic Light-Emitting Diode“
T. Grünbaum

15:50-16:10 O-9: „Magnetoconductance Study on Nongeminate Recombination in Solar Cell of rrP3HT and PC61BM“
T. Ikoma

Official poster session

16:10-18:10 Poster session

Tuesday, August 14

Session 5 (Session Chair: R. Coehoorn)

08:50-09:20 I-6: „Organic Biluminescence: An Emissive System With Both Fluorescence And Phosphorescence At Play“
S. Reineke

09:20-09:40 O-10: „Site-selective measurement of coupled spin pairs in an organic semiconductor“
A. Chepelianskii

09:40-10:00 O-11: „Detecting Singlet Transitions In Individual Molecules“
C. Meyer

10:00-10:20 O-12: „Temporal Mapping Of Excitonic Wavefunctions With Carbon Specificity“
A. Drew

Coffee break and posters

Session 6 (Session Chair: R. Kawakami)

10:40-11:10 I-7: „High quality factor spin wave resonances in organic-based ferromagnetic Vanadium Tetracyanoethylene“
N. Zhu

11:10-11:30 O-13: „Design, Syntheses and Photoconductivity of Pentacene-Radical Derivatives with Remarkable Photostability“
Y. Teki

11:30-11:50 O-14: „Patterning and Device Integration of Vanadium Tetracyanoethylene for Coherent Magnonics“
E. Johnston-Halperin

Lunch break and posters at Leopoldina

Session 7 (Session Chair: Z.-G. YU)

12:50-13:10 O-15: „Guiding Molecular Spintronics Design Using First-Principles Multi-Scale Modeling“
E. R. McNellis

O-16: Cancelled

13:10-13:30 O-17: „Magnetoresistance in organic semiconductors: Including pair correlations in the kinetic equations for hopping transport“
A.V. Shumilin

13:30-13:50 O-18: „Hot Electrons and Hot Spins at Metal–Organic Interfaces“
F. Ortmann

Coffee break and posters

Session 8 (Session Chair: E. Johnston-Halperin)

14:30-14:50 O-19: „The organic materials database - OMDB: a novel framework for functional materials prediction“
R. M. Geilhufe

14:50-15:10 O-20: „Simple Spintronics Based on Chiral Molecules“
Y. Paltiel

15:10-15:30 O-21: „Theoretical Characterization and Design of Organic Open-Shell Materials“
K. S. Schellhammer

Official poster session

Session 9 (Session Chair: E. Ehrenfreund)

17:00-17:30 I-8: „Magneto-Optical Properties and Coherent Spin Dynamics in Hybrid Organic-Inorganic Perovskites“
Z.-G. Yu

17:30-17:50 O-23: „Multiscale modeling of spin-relaxation in PBTTT“
U. Chopra

17:50-18:10 O-24: „Steric Effects on Spin-Orbit Induced Relaxation in Organic Semiconductors“
S. R. McMillan

Wednesday, August 15

Session 10 (Session Chair: A. Dediu)

08:50-09:20 I-9: „Long range lateral spin transport in conjugated organic polymers“
H. Sirringhaus

09:20-09:40 O-25: „Spin-Charge Conversion In the π-conjugated Polymer PBTTT“
M. M. Qaid

09:40-10:00 O-26: „Tuning Spin Injection by Molecular Design“
A. Wittmann

10:00-10:20 O-27: „Opportunities for Organic Spintronics in Waste Heat Harvesting“
C. D. W. Cox

Coffee break and posters

Session 11 (Session Chair: T. Moorsom)

10:40-11:10 I-10: „Geometry effects in spin pumping through thin organic films“
T. Richter

11:10-11:30 O-28: „A theoretical study of spin Hall effect in PBTTT“
M. R. Mahani

11:30-11:50 O-29: „Spin Pumping in Hybrid Organic-Inorganic Perovskite“
C. Nicolaides

11:50-12:10 O-30: „Effects of a Molecular C60 Interfaces on the Spin Hall Magnetoresistance of YIG/Pt“
S. Alotibi

Wednesday afternoon Excursion and Dinner

16:30-18:00 Boat tour on the River Saale

18:00-24:00 Bus transfer, guided tour and conference dinner at the Rotkäppchen Sektkellerei (champagne making facilities) in Freyburg

Thursday, August 16

Session 12 (Session Chair: Y. Teki)

08:50-09:20 I-11: „Strong Modulation of Spin Currents in Bilayer Graphene by Static and Fluctuating Proximity Exchange Fields“
R. K. Kawakami

09:20-09:40 O-31: „Spin Dependent Capacitance in a Metal-Oxide-Molecule Heterojunction“
T. Moorsom

09:40-10:00 O-32: „Anomaly transport in graphene and Weyl systems normally explained“
K. Morawetz

10:00-10:20 O-33: „Paramagnetic Meissner Effect in Metal-Molecule Hybrid Systems“
M. Rogers

Coffe break

Session 13 (Session Chair: A. Drew)

10:40-11:10 I-12: „Studying Spin Orbit Coupling in Organic Semiconductors“
C. Boehme

11:10-11:30 O-34: „Magnetic Dynamics and Order in the Lanthanide Single-Ion Molecular Magnets“
Z. Yang

11:30-11:50 O-35: „Spin Dynamics in High Mobility Conjugated Polymers“
S. Schott

11:50-12:10 O-36: „EPR Spectroscopic Signatures of C60 and C70 Fullerene Cations“
W. Harneit

12:10-12:30 Closing remarks

Departure

List of posters

P-1: „Controlling Triplet Excitations by Molecular Design“
A.A. Szumska

P-2: „TRESR and EDMR Study of Excitonic and Photocarrier Processes in Vacuum Vapor Deposition Film of Weak Charge Transfer Complex (II)“
K. Kato

P-3: „Magnetic Field Effects on Photocurrent in Organic Molecular Systems“
M. Klein

P-4: „Recombination Dynamics in P3HT:PC71BM Organic Solar Cell Studied by Magnetoconductance Effect“
R. Shoji

P-5: „Excitons in Topological Molecular Aggregates“
M. Shakirov

P-6: Cancelled

P-7: „Oscillating Spin Hall Effect in Organic Chains via Polaron Transport“
G. C. Hu

P-8: „Magnetic Field Effect on Pentacene-Doped Sexithiophene Diodes“
S.-T. Pham

P-9: Withdrawn

P-10: „MAGNETORESISTANCE IN ORGANIC SPIN-VALVE AT ROOM TEMPERATURE“
D.Dhanalakshmi

P-11: „Light induced magnetoresistance in solution processed planar hybrid devices measured under ambient conditions“
G. Salvan

P-12: „Magneto-conductance and Magneto-electroluminescence in High Magnetic Field in Organic Light Emitting Diodes“
D. Nikiforov

P-13: „TMR in Magnetic Tunnel Junctions with Phenalenyl-molecule Tunnel Barriers“
N. Jha

P-14: „Spontaneous spin polarization of methanol molecule adsorbed on B- or N-doped graphene: first-principles calculations“
J. F. Ren

P-15: „EPR Study of Spin Dependent Charge Transfer Processes at Functionalized Electrodes“
F. Blumenschein

P-16: „Ferroelectric control of organic/ferromagnetic spinterface“
Y. Lu

P-17: „Substitution effect on electronic and magnetic properties of double perovskite Sr2FeMoO6“
O. Sahnoun

P-18: „Easy-plane ferroborates. Magnetopiezoelectric effects“
T. Gaydamak

P-19: „Half-metallic completely compensated ferrimagnets in Cr doped BaP“
A. Bouabca

P-20: „Interlayer Exchange Coupling between Ferromagnetic Films through Topological Insulators“
S. Mehboodi

P-21: „Low Temperature Reflux Synthesis and Study of Cobalt Ferrite Nanoparticles“
B. Thombare

P-22: „Half metallic Fe3O4 thin films for organic spintronic“
M. Bohra

P-23: „Observation of Dzyaloshinskii-Moriya interaction in Co/Pt multilayers“
D.-H. Kim

P-24: Cancelled

P-25: „Integration of Molecular Quantum Bits with Organic Semiconductor Spintronics“
M. Kern

P-26: „Study of 12-Metallacrowns-4 Complexes“
S. Lach

Notes

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Abstracts

Signature of Exchange Bias and Room Temperature Magnetic Order in Molecular Layers

M. Gruber[1,2,3] , F. Ibrahim[1], S. Boukari[1], H. Isshiki[2], L. Joly[1], W. Wulfhekel[2],

F. Scheurer[1], W. Weber[1], M. Alouani[1], E. Beaurepaire[1] and M. Bowen[1]

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Hybrid samples, composed of a molecular layer sandwiched between two inorganic ferromagnetic (FM) layers, can exhibit sizeable magnetoresistance [1,2]. In such hybrid samples, the spin-dependent transport properties may be driven by the physics occurring at the metal-molecule interfaces also referred to as spinterface [2-5]. Separately, molecular semiconductor may exhibit antiferromagnetic (AF) correlations well below room temperature. Yet, surprisingly, while magnetic pinning of a FM layer through exchange bias with an AF layer constitutes a cornerstone of spintronics, this ingredient remains missing in molecular spintronics.

We performed X-ray magnetic circular dichroism measurements on paramagnetic manganese-phthalocyanine (MnPc) molecules deposited onto a FM Co(001) surface. The measurements, in combination with ab initio calculations, show that the Co/MnPc spinterface stabilizes an AF ordering at room temperature within subsequent MnPc monolayers away from the interface. In turn, we studied the impact of the AF MnPc layer on the Co substrate using the magneto-optic Kerr effect: the molecular AF layer magnetically pins the underlying Co film at temperatures below 100 K [5,6].

References

1. V. A. Dediu, *et al.*, Nat. Mater. **8**, 707 (2009)
2. C. Barraud, *et al.*, Nat. Phys. **6**, 615 (2010)
3. K. V. Raman, *et al.*, Nature **493**, 509 (2013)
4. F. Djeghloul, *et al.*, J. Phys. Chem. Lett. **7**, 2310 (2016)
5. M. Gruber, *et al*, Nat. Mater. **14**, 981 (2015)
6. S. Boukari, *et al.*, e-print arXiv:1712.07450 (2017)

Magnetic Subunits Within a Single Molecule-Surface Hybrid

D.E. Bürgler[1,4], V. Heß[1,2,4], R. Friedrich[3,4], F. Matthes[1,4], V. Caciuc[3,4],
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Magnetic molecule-surface hybrids [1] are ideal building blocks for molecular spintronic devices [2] due to their appealing tailorable magnetic properties and nanoscale size. So far, assemblies of interacting molecular-surface hybrids needed for spintronic functionality were generated by depositing aromatic molecules onto transition-metal surfaces, resulting in a random arrangement of hybrid magnets due to the inherent and strong hybridization. Here, we demonstrate the formation of multiple intramolecular subunits within a single molecule-surface hybrid by means of spin-polarized scanning tunneling microscopy experiments and ab-initio density functional theory (DFT) calculations [3]. This novel effect is realized by depositing the polycyclic aromatic triphenyl-trazine molecule comprising in total four aromatic rings onto two monolayers Fe on W(110). A highly asymmetric and chiral adsorption geometry induces different structural, electronic, and magnetic properties in each aromatic ring of the molecule. In particular, the induced molecular spin polarization near the Fermi energy is opposite to that of the Fe film and varies among the rings due to site- and spin-dependent molecule-surface hybridization. DFT calculations confirm the formation of multiple distinguishable magnetic subunits, each consisting of an aromatic ring and the Fe atoms directly underneath, with different magnetic moments and exchange coupling constants among each other and with respect to the unperturbed Fe environment as a consequence of their structural distinctiveness. Our results showcase a possible organic chemistry route of tailoring geometrically well-defined assemblies of magnetically distinguishable subunits with tunable magnetic interactions in a single molecule-surface hybrid.

References

1. M. Callsen *et al.,* Phys. Rev. Lett. **111**, 106805 (2013)
2. S. Sanvito, Chem. Soc. Rev. **40**, 3336 (2011)
3. V. Heß *et al.,* New J. Phys. **19**, 053016 (2017)

How to Probe the Spin Contribution to Momentum Relaxation in Topological Insulators

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Topological insulators exhibit a metallic surface state in which the directions of the carriers' momentum and spin are locked together. This characteristic property, which lies at the heart of proposed applications of topological insulators, protects carriers in the surface state from back-scattering unless the scattering centres are time-reversal symmetry breaking (i.e. magnetic) [1, 2, 3]. Experimental efforts to investigate this sensitivity of the surface state to magnetic scattering have so far focused on bulk doping topological insulators with magnetic defects [1, 2, 3]; in general this profoundly modifies the materials' electronic structures, impeding the interpretation of results and obfuscating the specific role of spin-momentum locking. We identify a new method of probing the effect of magnetic scattering by decorating the surface of topological insulators with molecules whose magnetic degrees of freedom can be engineered independently of their electrostatic structure [4]. We show that this approach allows us to separate the effects of magnetic and non-magnetic scattering in the perturbative limit [5]. We thereby confirm that the low-temperature conductivity of SmB_6 is dominated by a surface state and that the momentum of quasiparticles in this state is particularly sensitive to magnetic scatterers, as expected in a topological insulator.

References

1. Hasan, Kane, Rev. Mod. Phys. **82**, 3045 (2010)
2. Qi, Zhang, Rev. Mod. Phys. **83**, 1057 (2010)
3. Ando, J. Phys. Soc. Jpn. **82**, 102001 (2013)
4. Gatteschi, Sessoli, Villain, Molecular Nanomagnets (OUP, 2006)
5. Nam *et al.*, Nature Comms. **9**, 56 (2018)

Hybrid Materials Featuring Molecular Quantum Bits

J. van Slageren[1], M. Kern[1], S. Lenz[1], M.B. Casu[2], and S. Ludwigs[3]

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Molecular quantum bits are paramagnetic organic or metal-organic compounds in which coherent superposition states can be generated by means of pulses of electromagnetic (microwave) radiation. These systems may one day be employed in quantum information processing.

Over the past decade, we have investigated the properties of molecular quantum bits[1–3]. We have demonstrated that the quantum coherence time, i.e., the lifetime of the superposition state is limited by interaction with specific nuclear spins and that removal of these spins leads to a pronounced increase in this coherence time reaching the 100 μs regime[2]. Finally, we were able to predict the coherence decay quantitatively, based solely on the molecular structure[3].

In recent times, we have become interested in thin films of molecular quantum bits. For the quantum coherent manipulation, we have developed a special resonator for pulsed electron paramagnetic resonance investigations. We have studied thin layers of several types of molecular quantum bits prepared by UHV-deposition onto a variety of substrates. We have studied the spinterface by means of XPS techniques and the thin layers by electron paramagnetic resonance. Furthermore, we have developed hybrid materials consisting of molecular quantum bits and semiconducting polymers, with the aim of investigating the interaction between stationary molecular quantum bits and mobile charge carriers. Preliminary results will be presented.

References

1. C. Schlegel, **J. van Slageren***, M. Manoli, E.K. Brechin, M. Dressel, *"Direct observation of quantum coherence in single-molecule magnets", Phys. Rev. Lett.*, **101**, 147203 (**2008**).
2. K. Bader, D. Dengler, S. Lenz, B. Endeward, S.D. Jiang, P. Neugebauer, **J. van Slageren*,** *"Room Temperature Quantum Coherence in a Potential Molecular Qubit", Nat. Commun.,* **5**, 5304 (**2014**).
3. S. Lenz, K. Bader, H. Bamberger, **J. van Slageren**,* *Quantitative prediction of nuclear-spin-diffusion-limited coherence times of molecular quantum bits based on copper(II), Chem. Commun.*, **53**, 4477 - 4480 (**2017**).

Nonlinear light-matter interaction: from superconducting qubits to spins in diamond

Eyal Buks[1]

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Cavity quantum electrodynamics (CQED) is the study of the interaction between matter and photons confined in a cavity. In the Jaynes-Cummings model the matter is described using the two-level approximation, and only a single cavity mode is taken into account. The interaction has a relatively large effect when the ratio $E/\hbar\omega$ between the energy gap E separating the two levels and the cavity mode photon energy $\hbar\omega$ is tuned close to unity.

The talk is devoted to the study of the light-matter interaction in the nonlinear regime using three different CQED systems. In the first experiment a Josephson flux qubit serves as a two-level system and a superconducting resonator as the cavity [1]. We experimentally find that the cavity response exhibits higher order resonances (called superharmonic resonances) in the nonlinear regime when the ratio $E/\hbar\omega$ is tuned close to an integer value larger than unity. In the second experiment the interaction between a spin ensemble of diphenylpicrylhydrazyl (DPPH) molecules and a superconducting resonator is explored in the region where $E/\hbar\omega \gg 1$ [2]. We find that the cavity response is significantly modified when the spins are intensively driven close to their Larmor frequency. Retardation in the response of the spin ensemble gives rise to effects such as cavity mode cooling and heating. In the third experiment the interaction between localized spins in diamond (nitrogen-vacancy and nitrogen substitutional) and a superconducting resonator is studied [3]. We find that nonlinearity imposes a fundamental limit upon sensitivity of CQED-based spin detection.

References

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2. Hui Wang, Sergei Masis, Roei Levi, Oleg Shtempluk and Eyal Buks, Phys. Rev. A 95, 053853 (2017).
3. Nir Alfasi, Sergei Masis, Roni Winik, Demitry Farfurnik, Oleg Shtempluck, Nir Bar-Gill and Eyal Buks, arXiv:1711.07760.

Resistive bistability in organic spintronic devices and applications to neuromorphic computing

Alberto Riminucci[1], Robert Legenstein[2], Zhi-Gang Yu[3], Raimondo Cecchini[1,4],
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Despite the extensive research efforts devoted to the understanding of spin transport in organic semiconductors, key results, such as the Hanle effect, are still missing[1]. Many of the results in this field were obtained with the organic semiconductor (OS) tris(8-hydroxyquinoline)aluminum (Alq3). We have identified two distinct sets of devices, one with low resistance that shows spin valve magnetoresistance, and one with high resistance, with no magnetoresistance; the set a specific device belongs to does not depend on its thickness.

To understand the low resistance devices, that show magnetoresistance and resistive multistability we have expanded on the impurity band model[2]. In our devices we envisage oxygen to be the impurity and bistability is attributed its migration within the organic semiconductor/AlOx bilayer.

These devices can be used as a synapse for neuromorphic computing and can be used in several types of neural networks, from a simple single layer perceptron to spiking neural networks. The presence of magnetoresistance adds a unique tool to effect parallel, selective changes on the weight of synapses.

We tested the effectiveness on the learning process of neural network. We considered reward-based learning in an actor-critic framework. That is, the model consists of two networks. The actor network learns a policy, that is, a suitable action (output) y(x) for the current input x. The critic network learns the expected R(x) reward for this input. The critic network is used to improve learning of the actor network. In both cases, the nonlinear update has a significant advantage in terms of the speed at which the performance goal of a mean reward of 0.95 is reached.

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Direct evidence of spin injection in the HOMO/LUMO levels of a molecular material using a Spin-OLED device

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The generation of a non-equilibrium spin polarization in the conducting bands of metals and semiconductors is nowadays at the basis of most spintronic applications and devices, with the exception of tunnelling devices where a different physics takes place.

In molecular spintronics, a direct observation of spin injection from magnetic electrodes into the frontier electronic levels of a molecular semiconductor (i.e., to the HOMO and LUMO levels) is still missing [1,2]. To achieve this challenge we undertake here the successful fabrication of a spin polarized OLED device (in short spin-OLED). This multifunctional device acts at the same time as light-emitting device and as spin-valve. In this device an increase in the magneto-electroluminescence up to 2.4 % for the antiparallel configuration of the magnetic electrodes has been measured. This result is especially relevant since for this configuration the total current flowing through the OLED is reduced with respect to that for the parallel configuration due to magnetoresistance effects. Therefore, this result rules out the possibility of a coupling between current and luminescence since this will result in the opposite effect (more current leads to more light) [3]. It should be therefore attributed to an augmentation of the singlet excitonic branch with respect to the triplet one as a result of a spin polarization in the semiconducting layer. Interestingly, this spin polarization coexists with the absence of the Hanle effect. This result suggests that new physics is needed for the description of the spin-environment interactions in molecular solids.

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Abrupt Change of Ligand Fields During Formation of Molecular Contacts

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We have studied magnetic properties of single M(thd)$_2$ molecules (M = Co, Ni, Cu) on Cu$_2$N/Cu(001) by scanning tunneling microscopy. Inelastic spectroscopy at 30 mK reveals that the molecules have a very clear excitation signature, allowing a complete reconstruction of the spin Hamiltonian. Some of the molecules display a Kondo resonance.

When approaching the tip of the microscope towards the molecule, the tunneling current abruptly jumps to higher values indicating the sudden deformation of the molecule bridging the tunneling junction. This deformation has a strong effect on the ligand field, changing excitation energies and the composition of the ground state. By approaching the tip further, a smooth change of crystal field parameters is possible.

As the fast jump-to-contact rearranges the energy levels of these molecules, we believe that it would potentially allow to prepare superposition quantum states, a necessary requirement for quantum computing.

Nanoscale Studies of Organic Radicals: Surface, Interface, and Spinterface

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Organic thin films and organic/inorganic interfaces remained in the focus of extensive investigations for almost three decades. Surprisingly, in comparison with this extended work, little attention has been devoted to the deposition of organic radicals on a substrate. This might be due to the fact these materials are considered not stable enough for evaporation.

In this work [1], we demonstrate that it is possible to evaporate and deposit organic radicals onto well-defined surfaces under controlled conditions, without degradation. Using soft X-ray spectroscopies, performed also at synchrotrons, we investigate thin film processes, surfaces and interfaces at the nanoscale, when organic radicals are deposited on metal and metal oxide surfaces. We suggest how to design organic radicals bearing in mind the thermodynamic factors that govern thin film stability, with the purpose of obtaining not only a chemically stable radical, but also stable thin films. We investigate the thermal and air stability of the deposited films, and we explore the influence of the surface/radical chemical bond and the role of surface defects on the magnetic moment at the interface. Our work shows that the use of X-ray based techniques represents a powerful approach to reveal the mechanisms governing complex interfaces, such as radical/metal and radical/metal-oxide where it is important to describe both charge and spin behavior (spinterfaces). A deep understanding of stable radical/inorganic spinterfaces may open the way to use radicals in solid state devices, or as quantum bits with dedicated configurations, as proposed for other molecular quantum bits, or in spin-based electronics.

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Electric Field Mediated Coherent Spin Tuning in Antiferromagnetic Molecular Magnets

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The control of molecular spins using electric fields is particularly valuable for molecular spintronics because strong electric fields can easily be generated and shielded in within a small volume, allowing addressing individual spin-carrying molecules in a device [1]. Here, we demonstrate linear spin-electric field interactions in ensembles of inversion symmetry breaking antiferromagnetic molecular magnets using echo-detected electron spin resonance (ESR) experiments with the application of external pulsed electric fields. Coherent tuning of the molecule Hamiltonian was observed in two molecules, Cr_7Mn (S = 1) and Cu_3 (S = 1/2), showcasing that electric fields can be used for spin state manipulation in quantum information processing. We discuss the potential applications of using all-electric/electric-magnetic hybrid pulses in single-molecule devices.

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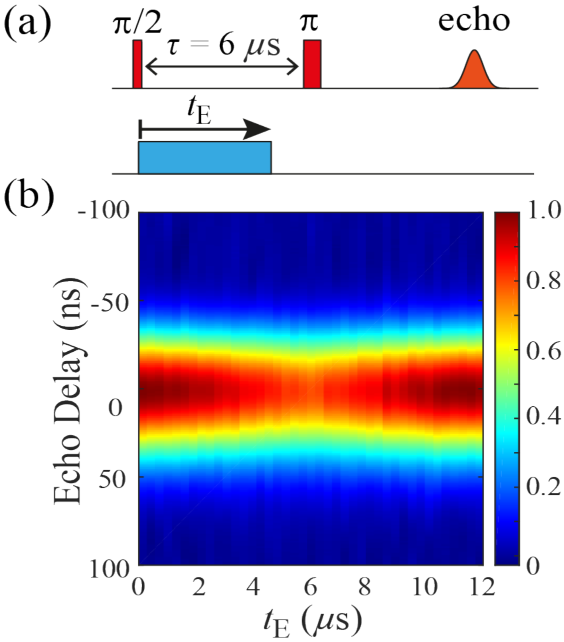

Figure 1: (a) The ESR (top) and electric field (bottom) pulse sequences. An electric field pulse was applied immediate after the π/2 pulse in the Hahn-echo sequence. The width of the electric pulse is varied from 0 to 2τ. (b) Spin echo signal for Cr_7Mn as a function of the electric field pulses. When $t_E = 2\tau$, the echo is identical to that without an external electric field, demonstrating coherent spin tuning of the spins by the electric field pulses.

Triplet interaction processes in phosphorescent and TADF-based OLEDs

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The efficiency of organic light-emitting diodes (OLEDs) is determined by a complex interplay between various interaction processes involving triplet excitons, such as triplet-triplet annihilation (TTA), triplet-polaron quenching (TPQ), triplet diffusion, and (reverse) intersystem crossing. Predictive OLED device modeling, using Kinetic Monte Carlo (KMC) simulations, requires disentangling all these processes. Whereas KMC modelling is now technically well feasible [1-3], the development of a proper experimentally validated mechanistic description of all relevant processes is still a subject of intense ongoing research. In this talk, first the state-of-the-art of three-dimensional KMC modelling of phosphorescent OLEDs is discussed, and an analysis is given of the sensitivity to assumptions related to TTA and TPQ, the processes leading to an efficiency loss at high current densities. Both processes are a result of the combination of a final interaction process and of diffusion processes (of excitons an/or polarons) that influence the overall loss rates. Experimental and simulation-based analyses of TTA and TPQ that enable disentangling these direct and indirect contributions are discussed. Finally, examples are given of applications of these results to TADF-based OLEDs.

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High Magnetic Field Effects in Organic Light Emitting Diodes

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Technion – Israel Institute of Technology

We have investigated magnetic field effects in low and high fields (B, up to 8 Tesla with high resolution of ~10^{-4} Tesla at low fields) over the temperature range 280-30 K in light emitting diodes made up of P3HT and super yellow (SY) organic semiconductors. In these devices we have measured magneto-conductance, MC, magneto-electroluminescence, MEL, magneto-photocurrent, MPC, and magneto-photoluminescence. At 280 K we find that the MC(B) and MEL(B) responses are identical (up to a B independent constant) and show near-saturation above B~1-2 T indicating that they are caused by identical species. However, at low temperatures they show different field dependent responses pointing toward the possibility of additional species that contribute to MEL(B).

In these low mobility substances magnetic field effects are attributed to the spin degrees of freedom. We explain the MC and MEL experimental results by studying the effect of magnetic field on polaron pairs composed of oppositely charged species with spin ½. In the low field regime (~10mT) the magnetic field effects are caused by the hyperfine interaction between the spins of the polarons and spins of the many protons that are present in all organic substances. In the intermediate field regime we consider a mechanism that was not discussed in detail previously and is caused by the anisotropy of the g-factor in these low symmetry organic molecules. The anisotropic g-tensor makes the levels containing the singlet S and triplet T_0 spin configurations vary with magnetic field, similar to the well-known Δg mechanism in devices where the positive and negative charges are on different molecules. In high fields (higher than 2 Tesla) we consider partial thermal spin polarization as an additional mechanism contributing to the magneto-effects. We have developed a simplified quantum mechanical approach taking into account the hyperfine and exchange interactions together with g-anisotropy and thermal effects. With this model we could account for the observed experimental data and draw conclusions about the exchange interaction between polarons that compose the polaron pair, the orientation of the g-tensors within the polaron pair in organic semiconductor and about the life time of polaron pairs in these organic light emitting diodes.

Electrical Detection of Ferromagnetic Resonance with an Organic Light-Emitting Diode

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Organic light-emitting diodes (OLEDs) constitute an ideal model system for investigating spin-dependent phenomena in condensed matter physics. A tool for direct access to the spin symmetry of charge carrier pairs in OLEDs is electron paramagnetic resonance [1]. Strong driving of the charge carrier spins by high frequency excitation reveals coherent phenomena such as the spin-Dicke effect [2] and the Bloch-Siegert shift.

Generating the high excitation fields necessary for these effects is experimentally challenging. One possible approach is to exploit high frequency magnetic stray fields originating from ferromagnetic resonance (FMR) in a proximate magnetic sample.

We investigate the effect of strong high frequency driving on a hybrid structure consisting of an OLED and a thin yttrium iron garnet (YIG) film. Under these conditions, an indirect bolometric effect enables the detection of the FMR driven in the YIG film in the DC resistance of the OLED. Good agreement of this electrically detected signal with FMR power absorption spectra is observed in Figure 1. The measurements reveal the bolometric nature of the signal, in agreement with earlier studies of electrical conductivity in magnetic thin films [3, 4].

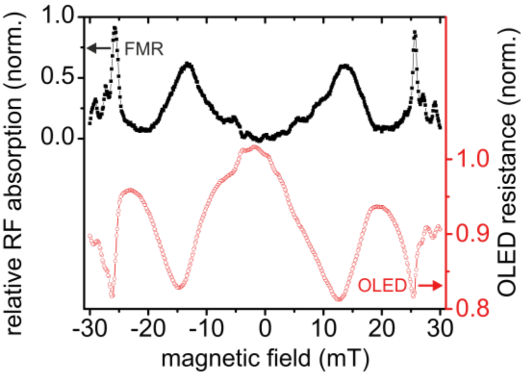

Figure 1: FMR absorption signatures in the DC resistance of an OLED.

We present a strategy to maximize the stray fields of the magnetic sample in order to enable large excitation fields for driving electron paramagnetic resonance in the OLED.

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Magnetoconductance Study on Nongeminate Recombination in Solar Cell of rrP3HT and $PC_{61}BM$

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It has been demostrated that magnetoconductance (MC) effect due to the hyperfine mechanism of geminate electron-hole (e-h) pair clarifies the carrier recombination yield of 1% in a single junction (SJ) solar cell consisting of pentacene and C_{60}.[1] In bulk junction (BJ) solar cells using regioregular poly(3-hexylthiophene) (rrP3HT) and [6,6]-phenyl-C_{61}-butyric acid methyl ester ($PC_{61}BM$), a similar positive narrow MC effect is observed in light. In addition broad MC effects due to the Δg mechanism of e-h pairs are also detected, which are negative below 1 T and positive above that.[2] It is pointed out that the inhomogeneous junction structure in BJ-cell affects the MC effect. In this paper, in order to elucidate the mechanism of the MC effect and the recobmination dynamics of e-h pairs, we measured the MC effects for SJ- and BJ-cells with rrP3HT and $PC_{61}BM$.

In magnetic field dependence of the MC effects observed in dark and light, there were three components with different half-field-at-half-maximums ($B_{1/2}$) of 5 ± 3, 30 ± 22 and > 400 mT, hereafter referred to $MC_{S, M, B}$ in a sequence. Magnitude of the $MC_{S, M, B}$ components was sensitive to not only the junction structure of cell but also the presence or absence of incident light. The bias voltage dependence of the dark MC effect and the light power and time dependences of the light MC effect clarified that all the three components were attributed from nongeminate e-h pair with spin-selective recombination. The sharp MC_S, middle MC_M and broad MC_B components are respectively derived from the hyperfine, spin relaxation and Δg mechanisms for the spin conversion of the ^{1,3}e-h pair. Kinetic simulations on the MC_S and MC_M components for the BJ-cell observed at the short-circuit condition in light indicate substantial nongeminate recombination that is accompanied with the generation of triplet exciton as well as the relaxation to ground singlet state.

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Organic Biluminescence: An Emissive System With Both Fluorescence And Phosphorescence At Play

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Organic molecules often make very good fluorescent emitters for which the exciton decay originates from their singlet states. On the contrary, radiative recombination from the triplet states is quantum mechanically forbidden, resulting in very weak radiative rates that are often much smaller compared to rates of non-radiative deactivation. Suppression of the non-radiative deactivation from the triplet states, which can be achieved by host:guest system engineering, will unlock this weak phosphorescence [1]. As a consequence, the organic luminophores turn into dual state emitters, which offer a direct spectroscopic access to both spin states and thus open up to a field of rich fundamental physics. This so-called biluminescence we discuss in this presentation with respect to the excitonic properties of such systems. In particular, a series of selectively brominated emitter molecules is discussed with respect to the internal mixing rate intersystem crossing, which defines the relative shares between singlet and triplet populations. Additionally, we discuss an energy transfer investigation involving a biluminescent donor paired with a fluorescent acceptor molecule resulting in simultaneous singlet and triplet transfer processes.

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Site-selective measurement of coupled spin pairs in an organic semiconductor

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From organic electronics to biological systems, understanding the role of intermolecular interactions between spin pairs is a key challenge. Here we show how such pairs can be selectively addressed with combined spin and optical sensitivity. We demonstrate this for bound pairs of spin-triplet excitations formed by singlet fission, with direct applicability across a wide range of synthetic and biological systems. We show that the site-sensitivity of exchange coupling allows distinct triplet pairs to be resonantly addressed at different magnetic fields, tuning them between optically bright singlet (S=0) and dark triplet, quintet (S=1,2) configurations: this induces narrow holes in a broad optical emission spectrum, uncovering exchange-specific luminescence. Using fields up to 60 T, we identify three distinct triplet-pair sites, with exchange couplings varying over an order of magnitude (0.3-5 meV), each with its own luminescence spectrum, coexisting in a single material. Our results reveal how site-selectivity can be achieved for organic spin pairs in a broad range of systems.

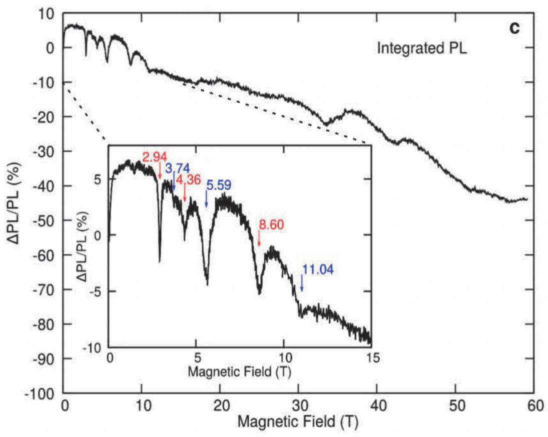

Figure 1: Photoluminescence in TIPS-tetracene at 2K as function of the magnetic field. Several resonancees with characteristic magnetic fields from 3 to 30 Tesla are seen which correspond to crossing between triplet/quintet and singlet states.

References:

arxiv.org/abs/1803.05225

Detecting Singlet Transitions In Individual Molecules

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Antiferromagnetic spintronics is an emerging field that holds great promise for technologies such as magnetic random access memories, neuromorphic computing and THz information technologies, because antiferromagnets (AFMs) do not produce and are insensitive toward magnetic stray fields [1]. Here, we show how concepts of antiferromagnetic spintronics can be applied to individual molecules. This is by no means trivial since currently used methods to measure molecular spin states rely on the detection of a local magnetic moment.

Here, we show that the switching between different $S = 0$ eigenstates of molecular complexes grafted covalently to carbon nanotube (CNT) quantum dots leads to a random telegraph signal (RTS) in the current through the devices (Figure 1).

The complexes contain either four Co^{II} or four Mn^{II} ions as spin-carrying species in a tetragonal core [2,3]. Analysing the statistics of the RTSs, we find that while Co^{II} complexes switch independently between states, the same complexes with Mn^{II} ions exhibit a *coherent superposition* between the states of all molecules attached to the quantum dot. We attribute this difference to the fact that in contrast to Mn^{II} ions, Co^{II} ions are prone to spin-orbit coupling, which is a known major source of decoherence. We find that a coherence time as long as seconds can be expected for antiferromagnetic states.

Our observations lead to a fundamentally new perspective for quantum computing with magnetic molecules: it appears very promising to search for molecules with different $S = 0$ states that can be used as quantum bits.

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Temporal Mapping Of Excitonic Wavefunctions With Carbon Specificity

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Organic semiconductors fall into a class of materials that shows significant potential for future applications, due to their ease of processing, low cost, highly tuneable electronic properties, favourable mechanical properties and long spin coherence times. Muon spin spectroscopy is a technique that has been applied to study a variety of intrinsic and device spin dynamics in organic systems [1-3], but little work has been done on exciton dynamics until recently, yet it's local nature is ideally suited to studying them [1]. I will discuss some recent results on exciton dynamics in TIPS-Pentacene [4], using the newly commissioned photo-musr setup on the ISIS HiFi spectrometer [5]. I will show that muons are sensitive to the time evolution of triplet excitons with a spatial resolution of individual and specific carbons on the backbone of the molecule, and discuss these results in the context of singlet fission.

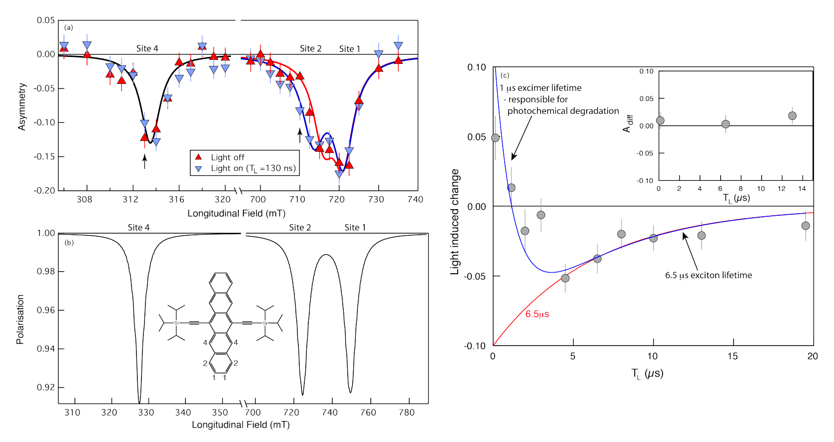

Figure 1: (a) Light induced changes to the muonium Avoided Level Crossing spectra for three different muonium bonding sites on the backbone of the molecule (see the inset to (b) for a diagram). Light induced changes are observed in the line shapes for only two of the three sites, corresponding to the end of the molecule. (c) The time dependence the light-induced signal for site 2, where two timescales can be seen. A signal corresponding to a dimer state (likely a singlet fission product, and a precursor to the final triplet excitation), and the triplet exciton lifetime, are observed.

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High quality factor spin wave resonances in organic-based ferromagnetic Vanadium Tetracyanoethylene

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The applications of long-lived spin wave excitations in magnetic materials have attracted intensive attention recently because of their high tunability and low ohmic loss. In particular, magnon-based transducers promise efficient, coherent, and low loss information storage and microwave signal processing. Although the recent magnonic devices are mainly based on inorganic ferrimagnet yttrium iron garnet (YIG), we demonstrate that the organic-based ferrimagnetic semiconductor V[TCNE]$_x$ (x~2, TCNE: tetracyanoethylene) is a compelling alternative to YIG due to its high Curie temperature (over 600 K), high quality (Q) factor spin wave resonance and excellent conformal chemical vapor deposition process on versatile substrates.

We realize integrated V[TCNE]$_{x\sim2}$ thin film microwave resonators patterned directly on sapphire chip at low temperature (50 °C). Spin wave modes are observed over a frequency range of 1 – 5 GHz with Q factors in excess of 3,200 under ambient conditions, rivaling the thin-film YIG devices grown epitaxially on lattice-matched GGG substrates. In 5-μm thick films, the Q factors of spin wave resonances are further enhanced over 8,000, and fine resonance spectra arising from geometry confined standing spin waves are resolved. These results establish the feasibility and potential of using V[TCNE]$_{x\sim2}$ thin films as a building platform for future integrated magnonic circuits.

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Design, Syntheses and Photoconductivity of Pentacene-Radical Derivatives with Remarkable Photostability

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Pentacene derivatives have been increasing interests as promising electronic materials of organic field-effect transistor (OFET) applications as the results of the high mobility. However, the photochemical instability in the presence of air prevents the practical application. We have, recently, discovered that a combination of two unstable species (photo-reactive pentacene and radical) leads to remarkable photochemical stability as well as solubility enhancement in common organic solvents [1,2]. We have also clarified that the ultrafast singlet-triplet conversion of the pentacene moiety by enhanced/accelerated intersystem crossing is the origin of the remarkable photo-stability [3].

In this work, we report the photoconductivity of the pentacene-biradical derivative, Pn(PhNN)$_2$ (Figure 1), investigated as a potential candidate of the organic spintronics materials. We have prepared polycrystalline films of the pentacene-biradical derivative on an interdigitated platinum electrode by a dip coating or a vacuum vapor deposition. The photocurrent was measured under a light illumination with Xe-lamp at room temperature. The radical moiety is sensitive for the external magnetic field and is also expected to act as an electron acceptor in the ground state or a donor in the excited state. We will also report the synthesis and physical properties of newly designed pentacene-radical derivative with a further improved photochemical stability.

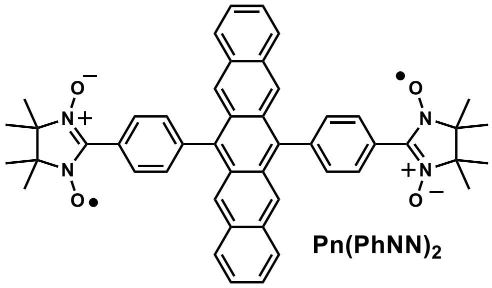

Figure 1: Pentacene-biradical

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Patterning and Device Integration of Vanadium Tetracyanoethylene for Coherent Magnonics

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The exploration of quantum magnonics relies implicitly on the ability to excite and exploit long lived spin wave excitations in a magnetic material. That requirement has led to the nearly universal reliance on yittrium iron garnet (YIG), which for half a century has reigned as the unchallenged leader in high-Q, low loss magnetic resonance and spin wave excitation despite extensive efforts to identify alternative materials. Recent work has identified the organic-based ferrimagnet vanadium tetracyanoethylene (V[TCNE]$_2$) as the first credible alternative to YIG. In contrast to other organic-based materials V[TCNE]$_2$ exhibits a Curie temperature of over 600 K with robust room temperature hysteresis with sharp switching to full saturation. Further, since V[TCNE]$_2$ is grown via chemical vapor deposition (CVD) at 50 C it can be conformally deposited as a thing film on a wide variety of substrates. Here we will discuss new approaches to patterning this material that meet the twin challenges of conformal CVD deposition and air/solvent sensitivity to achieve micro- and nano-scale patterning as well as device integration. These strategies maintain the high quality of the magnetic material, yielding quality factors ranging from 2,000 to over 8,000 in patterned structures. This patterning fidelity allows us to tune the spin-wave (magnon) excitation spectrum and to explore the strong coupling regime for magnon-magnon interactions within engineered nanostructures. In combination with low temperature CVD synthesis, these results demonstrate the unique ability to pattern on-chip high-Q magnonic structures with implications for emerging applications ranging from microwave electronics to quantum information systems.

Guiding Molecular Spintronics Design Using First-Principles Multi-Scale Modeling

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The vast tunability of molecular materials and components holds great potential for advances in spintronics. In real molecular materials, spin dynamics are governed by the interplay of a range of competing phenomena, including electronic spin-orbit coupling, local magnetic fields, electron dynamics, morphological and geometric effects etc. This complexity poses a great challenge for theoretical modeling.

We have developed a multi-scale modeling framework for microscopic spin dynamics in realistic material models. Starting from comprehensive first-principles theory for single to tens of molecules, we reach bulk material scales using state of the art tight-binding, stochastic and semi-classical models.

These techniques uniquely allow us to describe the subtle balance of influences on spin dynamics in various regimes, and to make quantitative predictions guiding experimental efforts to improve the design of molecular spintronics.

Along with an overview of our methodological challenges and developments, we will present results for the first few applications including fully first-principles spin dynamics in bulk Alq3, spin diffusion mechanics in several high-mobility polymer materials (e.g. spin diffusion in PBTTT), the CISS effect, and, more generally, the role and characteristics of molecular spin orbit coupling in molecular spintronic phenomena.

Magnetoresistance in organic semiconductors: Including pair correlations in the kinetic equations for hopping transport

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The organic magnetoresistance (OMAR) is known since 2005. Several qualitative mechanisms of OMAR were proposed and supported with Monte-Carlo simulations. However the existing approaches to its macroscopic theory look more like an artificial attempt to add the effect to the existing theories of hopping transport than like a consistent derivation of the theory.

In our work we focus on the reasons while the conventional theory of the hopping transport does not predict OMAR. We show that critical assumption is the Hartree decoupling. It disallows to include spin correlations into the theory and the spin degree of freedom appears to be reduced to averaged polarization of localization sites. However the known qualitative mechanisms suggest that OMAR is related to spin correlations and not to average polarization.

In our study we go one step beyond the Hartree decoupling. We include spin correlations in the simplest form, i.e. we include only pair correlations at close sites. We also consider simplified spin dynamics that is described with a single spin relaxation time. We show that even with these simplifications the connection between spin relaxation and the charge transport exists in the theoretical approach. Therefore OMAR can be described with the theory.

The dependence of the resistance on the applied magnetic field in our theory is controlled by the magnetic field dependence of the spin relaxation time as is essentially the same as in other approaches. However the dependence of magnetoresistance on system parameters is different. We show that the spin correlations are not generated in an ordered system with zero Hubbard energy leading to the absence of OMAR. The disorder or finite Hubbard energy re-establish the magnetoresistance.

Hot Electrons and Hot Spins at Metal–Organic Interfaces

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Metal-organic interface barriers can be investigated by energetic electrons [1], which are a promising probe also for spin dependent interface properties. A model is developed to describe the electron transport properties of hot electrons and hot spins in devices based on organic semiconductors [2]. For the first time, the simulations cover all the different processes the carriers experience in the device, which allows disentangling various effects on the transport characteristics. The model is compared to experimental measurements and excellent agreement is found.

As a second step, the model includes the electron's spin and is thus able to describe a hot spin transistor. In this device, a spatial variation of the spin diffusion length is found, which scales inversely proportional to the variation of the electron density. The spin current can be increased by increasing the hot electron energy and by decreasing the image charge barrier without changing the spin diffusion length. Unprecedented insight into the effect of interfacial disorder at the metal–organic interface on charge and spin transport is provided. Finally, conditions are established, where majority and minority spin carriers propagate in opposite directions, increasing the spin current relative to the charge current. The occurrence of pure spin currents is analyzed.

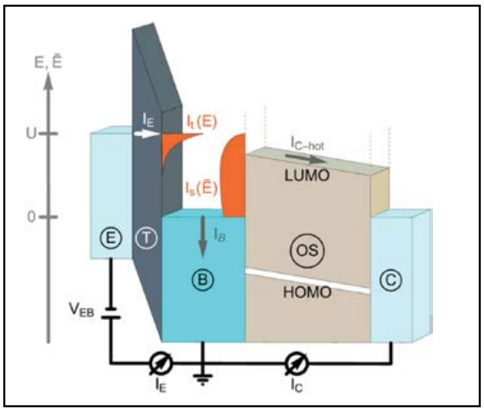

Figure 1: Schematic representation of the hot-electron device consisting of emitter (E), tunneling barrier (T), base (B), organic semiconductor (OS), and collector (C).

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The Organic Materials Database - OMDB: a Novel Framework for Functional Materials Prediction

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We present the organic materials database - OMDB, a freely accessible database for previously synthesized 3-dimensional organic crystals, available via *https://omdb.diracmaterials.org* [1]. The OMDB contains electronic and magnetic structure data calculated by us in the framework of the density functional theory. The web interface of the OMDB contains non-trivial search tools for the identification of novel functional materials such as band structure pattern matching [2] and density of states similarity search [3]. Currently, we implement state-of-the-art machine learning tools, e.g., for the prediction of material properties. We bring together scientists, publishers, and industrial partners of various backgrounds interacting via the OMDB. The OMDB community provides additional resources and services such as computational support, experimental verification and synthesis.

Additionally, we discuss our efforts in the design of organic topological semimetals and their tendency to establish symmetry breaking instabilities with localized spins. We furthermore report about our recent progress in calculating magnetic properties for the organic molecular crystals stored within the OMDB, such as local magnetic moments, Heisenberg exchange parameters and magnon spectra.

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Simple Spintronics Based on Chiral Molecules

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The high level of energy dissipation associated with the present semiconductor-based integrated-circuit technology limits the operating frequency of the devices. Therefore, there is interest in new concepts that may solve this problem. One such concept that attracts considerable attention nowadays combines spins with electronics (spintronics). In principle, the application of spintronics should result in reducing power consumption of electronic devices and efficiency should be closer to the thermodynamic limit.

Two major issues complicate the use of spintronics; material problems and the inefficiency in producing spin-polarized current. Spintronics devices usually require the use of complicated structures of magnetic material layers and the need for permanent magnetic layers puts constrains on the miniaturization of these devices. In addition, high currents are required to produce highly polarized spin current which results in induced heating.

We present a new concept in which spin current is produced by using the spin selectivity in electron transport through chiral molecules, termed Chiral-Induced Spin Selectivity (CISS)[1]. The CISS effect allows realization of simple local and power efficient spintronics devices. Studying the CISS effect, we found that chiral molecules, especially helical ones, can serve as very efficient spin filters at room temperature, with no need for a permanent magnetic layer. Recently, by utilizing this effect we demonstrated a simple magnetless spin based magnetic memory.[2-5] Moreover, we show that when chiral molecules are adsorbed on the surface of thin ferromagnetic film, they induce magnetization perpendicular to the surface, without the application of current or external magnetic field.[6]

The CISS-based spintronics technology has the potential to overcome the limitations of other magnetic-based memory technologies and to facilitate the fabrication of inexpensive, high-density memory and other spintronics elements.

Image

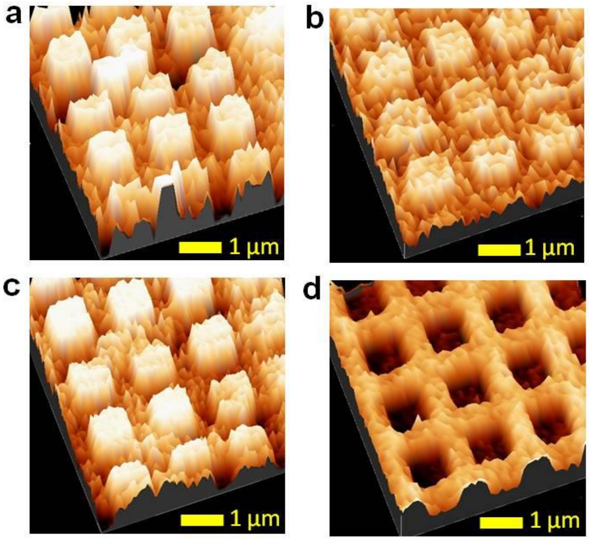

Fig. 1 | Topography and magnetic phase MFM images of a molecular induced magnetization orientation. AFM topography images of SAMs of AHPA-L **(a)** and AHPA-D **(b)** adsorbed on FM Co thin layers coated with a 5nm Au over-layer and their corresponding MFM molecular induced magnetic phase images of AHPA-L **(c)** and AHPA-D **(d)** magnetization orientation.

Recent Publications

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3) O. Ben Dor, N. Morali, S. Yochelis and Y. Paltiel "*Local Light-Induced Magnetization Using Nanodots and Chiral Molecules*" Nano Letters **14** 6042 (2014).
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Theoretical Characterization and Design of Organic Open-Shell Materials

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In recent years, organic molecules with stable open-shell ground states have attracted growing interest due to their outstanding properties, *i.e.* responsive spin structures, high-spin ground states, two-photon absorption, or small band gap. Although a growing number of interesting materials has appeared, molecules often lack in thermal stability impeding their application in spintronic devices.

In this presentation, we will highlight routes but also dead ends in the quest for high-spin configurations in hydrocarbons. We benchmark a computational approach based on density functional theory (DFT) and CASSCF for the analysis of open-shell organic structures, which combines predictability with appropriate simulation resources. For polycyclic heteroaromatic hydrocarbons containing a benzoisoindole core, we analyze singlet-triplet energy splittings and explain why a supposedly open-shell material does not provide the desired characteristics. [1] On the way towards possible quintet spin configurations, on the contrary, we discuss the promising characteristics of stable polycyclic hydrocarbon diradicaloids as well as related tetraradicaloids [2].

We demonstrate that significant optimization of material properties can be achieved already by chemical functionalization, while the full potential of promising material groups like bisphenalenyl-based molecules is far from being fully exploited.

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Magneto-Optical Properties and Coherent Spin Dynamics in Hybrid Organic-Inorganic Perovskites

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Hybrid organic-inorganic perovskites (HOIPs) have proven to be a revolutionary material for low-cost optoelectronic applications. They also exhibit novel magneto-optical effects [1] and surprisingly long spin coherence [2]. In this talk, I will show that many transport, excitonic, and spintronic properties in HOIPs can be systematically described by an effective-mass model [3] that predicts spin-dependent optical selection rules and *g*-factors of electron and hole spins, in addition to the electronic structure. In particular, this model relates the inversion-asymmetry parameter with the Rashba splittings of conduction and valences bands in HOIPs. The colossal Rashba effect is shown to qualitatively alter electrical transport [4], electron-hole recombination [5], and free-carrier absorption [6], as well as to result in the unusual spin relaxation behavior in HOIPs [7]. These results suggest that HOIPs have a great potential in spintronics.

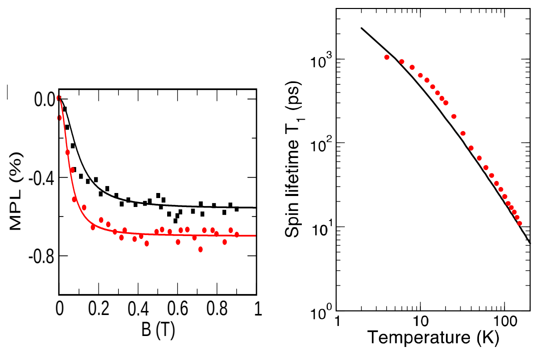

Figure 1: Magneto-PL for different photoexcitation intensities (left) and temperature dependence of spin lifetime (right).

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Multiscale modeling of spin-relaxation in PBTTT

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Among potential candidates for organic spintronics, the chalcogenide class of polymers are particularly interesting due to their unconventionally high charge mobility [1]. Recent experiments show that semi-crystalline PBTTT can conduct pure spin-currents with spin-diffusion lengths that spans hundreds of nm [2]. However, there is no previous theoretical model which treats spin transport in the polymer from first-principles. In this work, we explore the effects of spin-relaxation mechanisms modelled using state-of-the-art first-principles techniques, on top of charge dynamics from multiscale modelling. For the latter, we use the VOTCA-CTP [3] package, and a PBTTT morphology obtained using MD. Our model considers hyperfine fields, spin-spin exchange and dipole interactions, spin-orbit coupling [4], and vibron assisted spin-relaxations. Our preliminary results explore spin-transport in an effectively one-dimensional transport along the $\pi-\pi$ stacking direction of the polymer. We find that all the spin-relaxation mechanisms are weak in PBTTT and spin-transport is highly sensitive to the spin-admixture parameter (γ^2) (SOC) [4] because of extremely high charge-hopping rates. We also find that transport is strongly influenced by exchange and dipolar interactions at higher carrier concentrations.

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Steric Effects on Spin-Orbit Induced Relaxation in Organic Semiconductors

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Organic semiconductors are desirable candidates for spintronic application due to their remarkably long spin relaxation times and weak intrinsic magnetic interactions. For typical pi-conjugated polymers the coupling between the spin-orbit interaction and low transport rates has exploitable consequences on the spin and charge dynamics when considering the impact of site orientation. In this work we use a continuous-time random walk model to predict the dependence of spin relaxation on the relative orientation between nearest neighbor sites. We consider the carriers to be non-interacting and the transport to occur as incoherent hops from one site to the next. This quantum mechanical investigation was adapted from earlier work [1]. Considering the inter-site orientation to be governed by thermal activation we establish a distribution, $P(\theta) \propto \exp(s_H \cos\theta)$, and quantify the degree of steric hindrance through the temperature dependent characteristic orientation of the distribution, $s_H = U_0/k_BT$, where U_0 is the maximum difference in steric potential between two sites. This allows the investigation of spin-relaxation as a function of steric constraint. Our results approach previously derived values [2,3] if we consider large coordination numbers under zero constraint. In the case of large constraint, we predict complete quenching of the spin-orbit relaxation mechanism. This result suggests the ability to tune the spin-orbit induced relaxation allowing for spin lifetime optimization for spintronic applications.

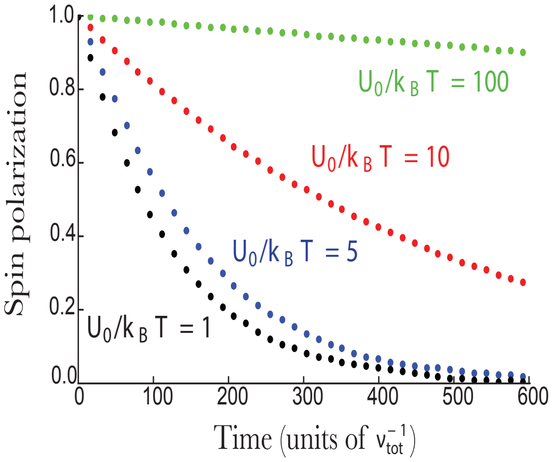

Figure 1: Spin polarization vs time for different steric hindrance constants in a unidirectional linear geometry. Large steric constant, U_0/k_BT, implies little variation in molecular orientation from site to site, drastically reducing the spin-orbit induced relaxation.

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Long range lateral spin transport in conjugated organic polymers

Shu-Jen Wang[1], Deepak Venkateshvaran[1], Erik McNellis[2], Uday Chopra[2], Reza Mahani[2], Angela Wittmann[1], Riccardo Di Pietro[3], Guillaume Schweicher[1], Keehoon Kang[1], Murat Cubukcu[1], Thomas J. Wagner[3], Cameron Jellet[4], Mark Little[4], Iain McCulloch[4], Joerg Wunderlich[3], Jairo Sinova[2], and Henning Sirringhaus[1]

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Over recent years there has been tremendous progress in developing low-temperature, solution-processible organic semiconductors that provide high charge carrier mobilities for both n-type and p-type device operation, good operational stability and other functionalities such as efficient electroluminescene, sensing or memory functions for a variety of applications. Here we are interested in understanding the spin physics of these materials and the relationship between molecular structure, microstructure and spin transport and relaxation. Organic semiconductors may enable realisation of long spin relaxation times and long spin diffusion lengths due to the weak spin-orbit coupling but it is difficult to achieve efficient spin injection by conventional electrical injection from spin-polarised ferromagnetic metals due to impedance mismatch. We have developed a method for efficient injection of pure spin currents into these highly resistive materials based on the technique of spin pumping using ferromagnetic resonance induced at the interface between ferromagnetic metals or insulators and organic semiconductors. This provides us with a powerful method for studying the spin physics and has enabled us to observe, for example, evidence of Hanle precession of spin polarised electrons in an organic semiconductor.

Spin-Charge Conversion In the π-conjugated Polymer PBTTT

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Spin pumping can be used to inject a pure spin current from a ferromagnet into a conducting non-magnet. By the inverse spin-Hall effect (ISHE) this spin current can be converted into a charge current, an effect also dubbed spin-charge conversion. We have investigated the ISHE in the π-conjugated polymer poly (2,5-bis (3-hexadecylthiophen-2-yl) thieno [3,2-b] thiophene) PBTTT doped with F4TCNQ. The material is deposited on a ferrimagnetic yttrium iron garnet (YIG) thin film. In ferromagnetic resonance a spin current is injected from the YIG into the PBTTT and the inverse spin-Hall effect can be measured in the organic semiconductor. We have investigated the ISHE for different PBTTT thicknesses and also for samples which were annealed in order to change the doping. For our measurements we have used a dedicated geometry which allows to measure very small ISHE signals without artifacts [1]. In addition we have excluded the Nernst effect which can be induced by thermal gradients caused by the RF excitation. We will present the results of the various ISHE measurements and discuss the possible side effects and their magnitude.

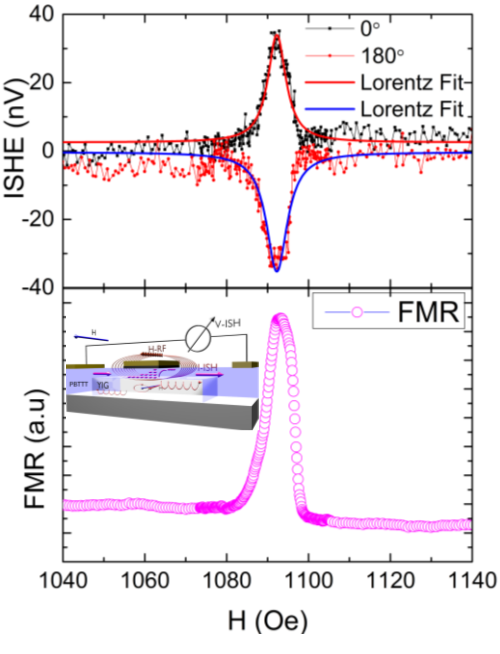

Figure 1: ISHE (top) measured at the same position of FMR (below). The inset below shows the schematic configuration used in our ISHE investigation.

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Tuning Spin Injection by Molecular Design

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Organic semiconductors have recently been found to have a comparably large spin diffusion time and length [1]. This makes them ideal candidates for spintronic devices.

The efficiency of spin injection at ferromagnetic resonance (FMR) from a ferromagnetic material (FM) into an adjacent non-magnetic material (NM) is given by the spin mixing conductance g_{eff}. It can be quantified by measuring the linewidth broadening of the FMR absorption of the FM due to an increase in Gilbert damping caused by spin injection into the NM. Here, we use this technique to systematically study spin injection from a metallic ferromagnet, $Ni_{80}Fe_{20}$, into organic semiconductors and directly demonstrate spin injection into small molecules and conjugated polymers. In particular, we investigate the influence of the molecular structure at the interface on the spin injection efficiency. One of the best performing small molecule organic semiconductors to date is dinaphtho [2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNTT)[2]. Comparing three derivatives of DNTT (chemical structure shown in figure 1a), we observe a significant suppression of the linewidth broadening (see figure 1b) and a decrease in spin diffusion length in C8-DNTT, which can be attributed to a larger separation of the core of the molecule from the interface due to the addition of alkyl side-chains. This demonstrates that both spin mixing conductance as well as the spin diffusion length can be tuned through molecular design.

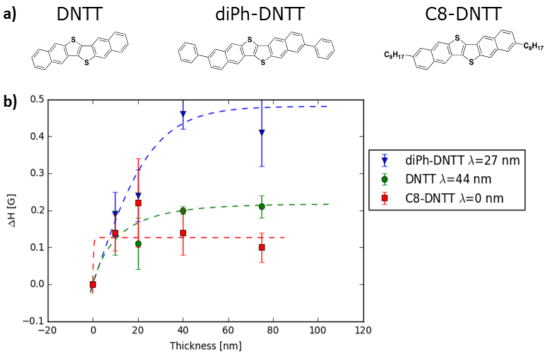

Figure 1: a) Chemical structure of three derivatives of DNTT b) Linewidth broadening as a function of thickness of DNTT (circles), diPh-DNTT (triangles) and C8-DNTT (squares). From the gradual increase in signal with film thickness, the spin diffusion length can be estimated for DNTT and diPh-DNTT using the fit (dashed line)

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Opportunities for Organic Spintronics in Waste Heat Harvesting

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The spin Seebeck effect (SSE), originally realised in 2008 [1], is a thermoelectric phenomenon defined as the establishment of a spin current due to the application of a temperature gradient across a material (see Figure 1). The SSE now governs the thermal generation of spin currents in a multitude of materials from ferromagnetic metals (Fe_3O_4 [2,3]), insulators (such as YIG [4]), antiferromagnets (MgF_2 [5]) and non-magnetic semiconductors (e.g. InSb [6]). The search for alternate material systems to investigate the interplay between thermal and spin currents is still full of vitality with the field of organic semiconductors now in the spotlight.

Recently an enhancement in the SSE signal has been found in the YIG/C_{60}/Pt system [7], paving the way for a combination of the fields of spin caloritronics and organic semiconductors.

We present our work on a variety of material systems including ferromagnetic metals and insulators and the measurement capabilities of our group.

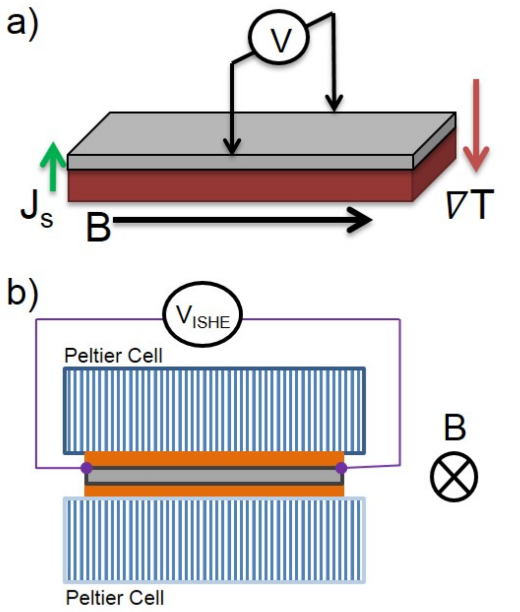

Figure 1: a) Geometry of the spin Seebeck effect in a FM/NM bilayer and (b) a typical measurement set up - sample clamped between two peltier cells. The inverse spin Hall voltage (VISHE), which is proportional to the SSE, is measured as a function of heat flow.

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Geometry Effects in Spin Pumping Through Thin Organic Films

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We investigate spin pumping from yttrium iron garnet (YIG) into Pt through ultrathin organic films (C_{60}, DH4T) of thicknesses d_0 between 0 and 10 nm. For all samples damping in ferromagnetic resonance (FMR) by spin pumping and the DC inverse spin-Hall effect (ISHE) in the Pt are measured. With increasing d_0 the damping drops monotonically from a maximum for zero interlayer thickness to zero for 10 nm or more. The ISHE, however, shows a non-monotonic behaviour. Maximum ISHE is observed for d_0=0. For d_0 of 1 or 2 nm the ISHE drops to less than 50% (Fig. 1). Further increase in d_0 leads to a reversal of this trend for both organic molecules and only after a second maximum is reached the ISHE drops to zero approx. exponentially with interlayer thickness. This surprizing result is caused by the growth mode of the organic layers. In very thin films the organic molecules form islands which can ideally be regarded as half spheres. Magnitude and direction of the ISHE depend on the absolute directions of pumped spins and spin current and their relative orientation. The spin current enters through the bottom of the islands but exits perpendicular to the organic/Pt interface. Only the spin current through the top of the island causes a maximum signal while currents flowing almost in plane barely contribute. They either do not cause any ISHE or they cause an ISHE which is perpendicular to the measurement direction. Thicker layers are almost closed and all spin currents again pass the interface perpendicular to the layer. So the original effect is restored, except for a decrease by spin flip in the organic film. Simulations and transmission electron microscopy show that this model fully describes our findings. The results are important because they show that especially for spin pumping through very thin films the morphology is extremely important and many different layer thicknesses need to be investigated to get a coherent picture. Due to the purely geometrical origin the effect is universal for all conducting interlayer materials.

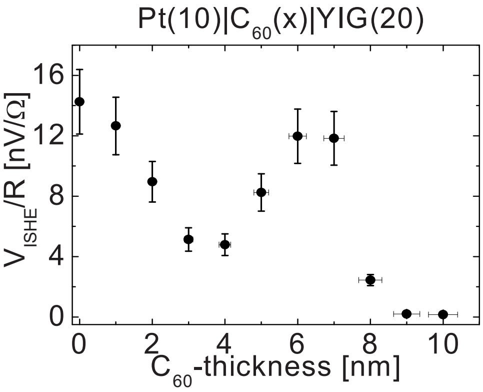

Figure 1: Dependence of ISHE on C_{60} interlayer thickness d_0.

A theoretical study of spin Hall effect in PBTTT

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The spin Hall effect (SHE), a direct conversion between electronic and spin currents, in organics has drawn great attention in the past few years. It relies mainly on the coupled motion of electrons to their spins due to the spin-orbit coupling (SOC), which is relatively weak in many organic materials. However, it has been recently shown that the SHE could arise at the first order of SOC where it originates from the misalignment of pi-orbitals in triads consisting of three molecules [1].

The importance of triads in the hopping transport regime was recognized earlier in the study of the Hall effect [2] and later in the study to obtain a general formula for the anomalous Hall conductivity [3].

Here, as part of a multiscale modeling, we describe the spin Hall effect in poly(2,5-bis(3-alkylthiophen2-yl)thieno[3,2-b]thiophene), (PBTTT) a thiophene-based conjugated polymers with high charge-carrier mobility. By extracting parameters directly from our first principle calculations, and based on the key aspects mentioned above, we calculate the electrical and spin hall conductivities for PBTTT.

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Spin Pumping in Hybrid Organic-Inorganic Perovskite

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Hybrid organic-inorganic perovskite materials have recently been attracting particular attention as an exceptional solar cell material. These compounds have been predicted to have large spin-orbit coupling [1], spin-dependent optical selection rules [2, 3] and are therefore a promising candidate family of materials for spintronics applications.

Here we present an experimental demonstration of spin transport at room temperature in solution processed $CH_3NH_3PbI_{3-x}Cl_x$ films. We have employed spin pumping under ferromagnetic resonance (FMR) in a microwave cavity for a series of $CH_3NH_3PbI_{3-x}Cl_x$/NiFe heterostructures with varying NiFe thicknesses deposited by e-beam evaporation. The evolution of the ferromagnetic layer as a function of its thickness was investigated by magneto-optic Kerr effect and AFM, showing a transition from island growth to percolation and finally to a formation of a polycrystalline NiFe thin film.

The generated spin current is detected as an additional broadening of the spectral width of the NiFe FMR absorption. By taking into consideration two-magnon scattering and inhomogeneity contributions to the obtained spectral width, the effective damping parameter, α_{eff}, has been calculated for every sample allowing us to extract the spin mixing conductance, $g^{\uparrow\downarrow} \approx 10^{19}\ \mathrm{m}^{-2}$ which is comparable with other metal/ferromagnet interfaces, suggesting that spin pumping by FMR is an efficient method to inject spin currents in perovskites for spintronic applications.

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Effects of a Molecular C_{60} Interfaces on the Spin Hall Magnetoresistance of YIG/Pt

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Spin Hall magnetoresistance (SHMR) is generated when a current passes through a thin (~nm) heavy metal layer with a large spin orbit coupling (SOC) deposited on a ferrimagnetic insulator. A spin current is generated in the metallic layer, perpendicular to the electronic current. When the direction of the magnetisation M in the ferrimagnet is parallel to Js, the spin current is reflected from the interface and back into the metal due to the inverse spin Hall Effect. However, if the direction of the magnetisation M and spin polarisation are perpendicular, the spin current is able to pass into the insulator by a spin torque and continue as a spin wave. Thus SHMR can be observed by rotating the magnetisation vector. This effect has generated a large interest over the last few years and it is critical in the study of the spin Hall angle and its applications, e.g. for devices such as spin torque MRAM [1, 2].

At molecule/ metal interfaces, the electronic properties are changed by hybridisation. For C_{60}/ transition metal interfaces a conducting interface and changes to the SOI of the metal can occur. Previously, it has been shown that this can lead to the emergence of spin ordering in interfaces with thin layers of transition metals.[3]. The interfacial effect is also critical in spin filtering and spin transport effects.[4]. This study is on the effect of C60 on SHMR. We aim: i. to maximise the SHMR for smaller metalic layers, and ii. to investigate the effect of C60 on the SOI of heavy metals. We find that the conducting interface formed between C_{60} and Pt layers of 1.5-3 nm reduces the resistance of the metal by 40-60%, with larger changes at lower temperatures. The SHMR and the anisotropic magnetoresistance (AMR) in the thicker Pt layers (~3nm) is reduced by approximately the same percentage see Fig.1. However, in the thinner Pt (~1-2 nm), the C_{60} protects the metal from oxidation and leads to larger magnetoresistive effects.

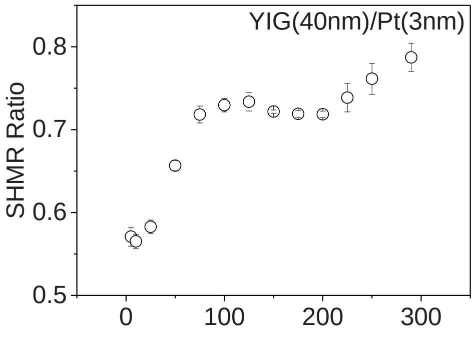

Figure 1: Ratio of the SHMR for Pt on YIG measured with and without a C_{60} layer on top at different temperatures.

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Strong Modulation of Spin Currents in Bilayer Graphene by Static and Fluctuating Proximity Exchange Fields

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Two dimensional (2D) materials provide a unique platform to explore the full potential of magnetic proximity driven phenomena, which can be further used for applications in next generation spintronic devices. Of particular interest is to understand and control spin currents in graphene by the magnetic exchange field of a nearby ferromagnetic material in graphene/ferromagnetic-insulator (FMI) heterostructures. Here, we present the experimental study showing the strong modulation of spin currents in graphene layers by controlling the direction of the exchange field due to FMI magnetization [1]. Owing to clean interfaces, a strong magnetic exchange coupling leads to the experimental observation of complete spin modulation at low externally applied magnetic fields in short graphene channels. As shown in Figure 1, when the FMI magnetization if parallel to the electron spin orientation, the spin current is allowed to reach detector. However, when the FMI magnetization is perpendicular to the electron spin orientation, the spin current is lost because of precessional spin dephasing due to the proximity exchange fields from the FMI. Additionally, we discover that the graphene spin current can be fully dephased by randomly fluctuating exchange fields. This is manifested as an unusually strong temperature dependence of the non-local spin signals in graphene, which is due to spin relaxation by thermally-induced transverse fluctuations of the FMI magnetization.

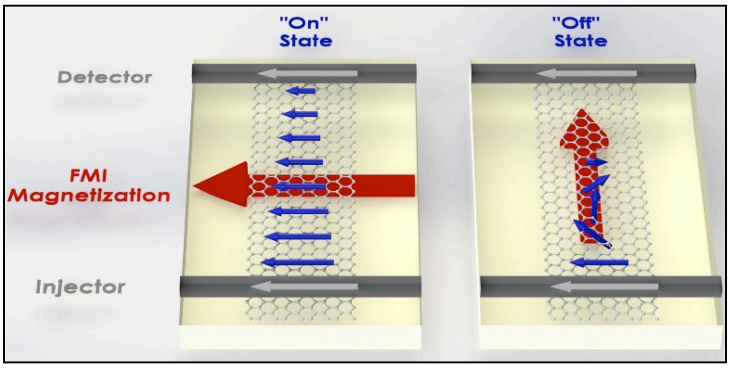

Figure 1: Modulation of spin current by proximity exchange fields from FMI underlayer. Parallel orientation (left) allows spin current to reach the detector, but perpendicular orientation (right) does not.

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Spin Dependent Capacitance in a Metal-Oxide-Molecule Heterojunction

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Producing devices based on active control of spinterface effects is the next major challenge facing molecular spintronics. [1] Spinterface control of ferromagnetism, spin texture and topological states have all been demonstrated. [2][3] However, there are persistent challenges associated with developing good quality gate contacts for molecular devices.

We demonstrate a two terminal device comprising a C_{60} film between manganate and transition metal electrodes, which exhibits spin dependent capacitance due to a spin filtering, polar interface. We also show how such a device might be controlled through the coupling of charge and ion currents to create a programmable spin filtering system where the spinterface is controlled chemically through displacing oxygen ions.

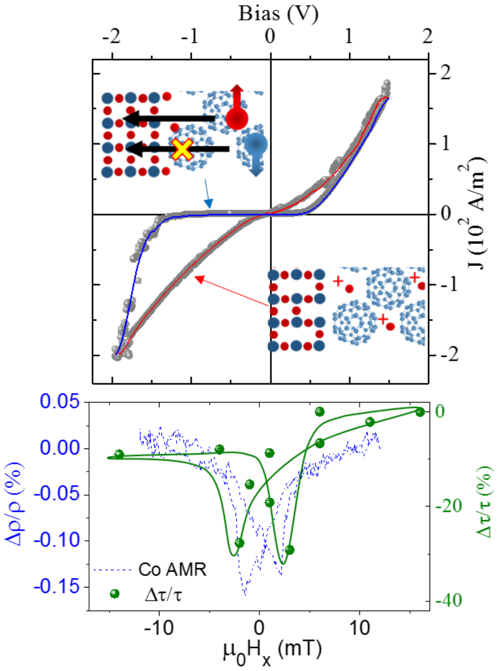

Figure 1: [TOP] I:V for a MnO/C_{60}/Co diode before (blue) and after (red) switching with a programming voltage. [Bottom] Discharge time constant of the diode as a function of field (green) overlayed on the AMR of cobalt electrode (blue).

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Anomaly transport in graphene and Weyl systems normally explained

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The quantum kinetic equation for systems with SU(2) structure is derived with special consideration of spin-orbit coupling in magnetic and electric fields. Chiral anomal transport is found to be derivable from a conserving theory without violation of conservation laws. Regularization-free density and pseudospin currents are calculated in graphene and Weyl-systems realized as the infinite-mass limit of nonrelativistic electrons with quadratic dispersion and a proper spin-orbit coupling. Correspondingly the currents possess no quasiparticle part but only anomalous parts. The intraband and interband conductivities are discussed. The optical conductivity agrees well with the experimental values using screened impurity scattering and an effective Zeeman field. The universal value of Hall conductivity is shown to be modified due to the Zeeman field. The pseudospin current reveals an anomaly since a quasiparticle part appears though it vanishes for particle currents. The density and pseudospin response functions to an external electric field are calculated. A frequency and wave-vector range is identified where the dielectric function changes sign and the repulsive Coulomb potential becomes effectively attractive allowing Cooper pairing. The coupled density and spin response functions allow to describe dynamical classical, quantum, and anomalous Hall effect as well as spin-Hall effects and its inverse.

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Paramagnetic Meissner Effect in Metal-Molecule Hybrid Systems

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Magnetism and superconductivity are competing phenomena, yet they are able to coexist due to the formation of spin-triplet Cooper-pair states [1]. Fullerene C_{60} is diamagnetic and insulating. However, its large electron affinity and low LUMO can lead to considerable charge transfer into the molecule from metallic surfaces. It has been shown that for metal/C60 interfaces, significant charge transfer and orbital hybridisation can lead to emergent spin polarised interfaces and ferromagnetic ordering [2]. Here, we show that in Nb/C60/Au systems, cooper pair leakage leads to a proximity induced SC state in the C60 with a coherence length, ξo, of 30±8 nm. Probing the local magnetic field distribution by Low Energy Muon Spin Rotation (LE-μSR), we observe conventional diamagnetic Meissner screening in a Nb/C60/Au stack extending into the Au layer. In a similar structure including a weakly magnetic C_{60}/Cu/C_{60} layer the diamagnetic screening in the Nb is slightly supressed whereas the screening in the Au is now paramagnetic. In some hybrid SC/FM structures such effects have been attributed to the generation of odd-frequency triplet cooper pairs [3]. Our initial results demonstrate the potential for forming unconventional cooper pairs in systems that contain no intrinsic exchange splitting and instead rely on the emergent effects that occur at molecule/metal interfaces.

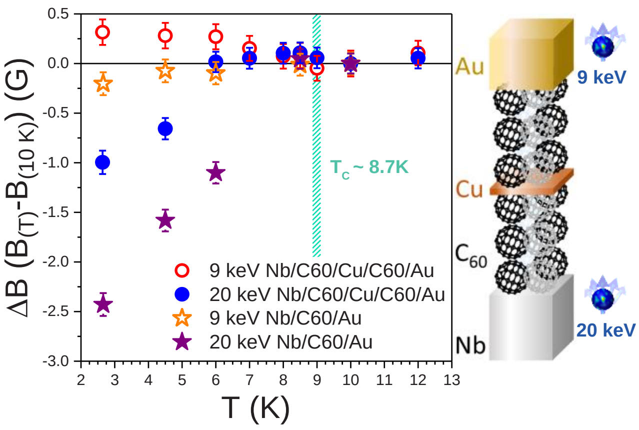

Figure 1: LE-μSR data showing diamagnetic screening in Nb (20keV) but opposite screening effects in Au layers (9keV) when a magnetic Cu layer is present.

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Studying Spin Orbit Coupling in Organic Semiconductors

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The role of charge carrier spin-orbit coupling (SOC) strength in organic and other predominantly carbon-based materials is considered to be negligible for many physical behaviors that these materials exhibit due to the strong dependence of the SOC on the atomic number. In recent years though, a variety of magnetoelectronic and spintronic material effects such as the high-magnetic field magnetoresistance behavior [1] and the inverse spin-Hall effect [2] have been reported to directly depend on SOC strength. In order to understand these phenomena, experimental methods to gain direct experimental access to charge carrier SOC are therefore needed. This presentation is focused on recent progress on electrically detected magnetic resonance (EDMR) schemes that were developed specifically to probe charge carrier Landé *g*-factors of weakly SOC systems. Effective *g*-factors of paramagnetic states are directly determined by SOC strengths and using EDMR to identify SOC induced spectroscopic shifts ensures that only electronic states are probed that significantly contribute to conductivity. However, there are challenges associated with this experimental approach: (i) the proton induced random local magnetic hyperfine fields in organic semiconductors usually dominate *g*-factor shifts in EDMR spectra, (ii) charge carrier wave function and associated *g*-factor anisotropies can cause convoluted and hard to analyze EDMR powder spectra and equally, (iii) the complexity by which *g*-factors are governed by SOC makes the analysis of SOC using EDMR spectra difficult. To solve these problems, high magnetic field EDMR (order of 10T) spectroscopy was developed where *g*-factor line broadening effects exceed typical hyperfine fields, and equally, data analysis techniques were developed using numerical models to describe paramagnetic charge carrier states and density functional theory to simulate resulting *g*-factor distributions that could be tested with experimental data [3].

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Magnetic Dynamics and Order in the Lanthanide Single-Ion Molecular Magnets

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A series of rare-earth metal containing molecules CP*-RE-COT (where RE represents Dy, Ho, Er, and Tm), known as single-ion molecular magnets (SIMMs), are investigated. The lanthanide ion is sandwiched by the $C_8H_8^{2-}$ (COT) and the $C_5Me_5^-$ (CP*) carbon rings [1]. Of interest is the low dimensionality of the magnetic properties, with only one large spin center carried by the rare-earth ion. A large magnetic anisotropy is attributed to the bending of the two carbon rings off the center and to the strong spin-orbit coupling.

As a result of the large relaxation energy barrier, CP*-RE-COT is expected to present a high blocking temperature. The spin multiplies experience further zero-field splitting by the crystal field, which makes it a rather complicated but very interesting problem [2]. Thermally activated magnetisation has been revealed, and the absence of slow relaxation is explained by the fast quantum tunneling of magnetisation (QTM).

We have studied the magnetic properties in CP*-RE-COT using both muon spin relaxation (μSR) and magnetometry measurements. The magnetisation relaxation rates are described by a combination of the Orbach and QTM processes. Most interestingly, the Dy complex is observed to exhibit long-range order (LRO) below the T_C (1.8 K). Our calculations suggest the presence of antiferromagnetic couplings with exchange J ~ -1.3 cm^{-1}.

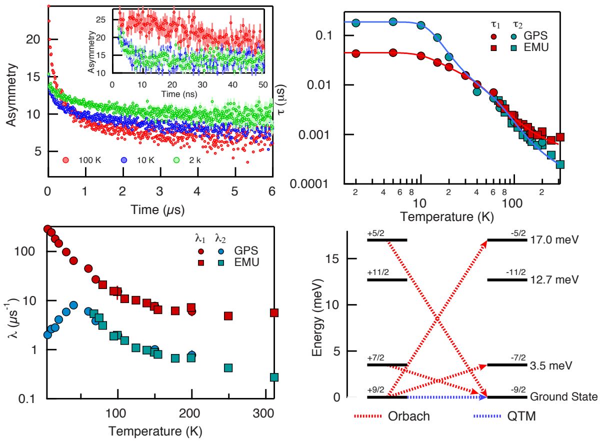

Figure 1: μSR data measured on CP*-Dy-COT: The muon spin relaxation rates vs temperature is obtained. And the magnetisation relaxation is distributed to the Orbach and QTM processes.

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Spin Dynamics in High Mobility Conjugated Polymers

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Polymeric semiconductors and conductors are enabling flexible, large-area optoelectronic devices, such as organic light-emitting diodes, transistors, and solar cells. Due to their exceptionally long spin lifetimes, these carbon-based materials could also have an impact on spintronics [1].

Weak spin orbit- and hyperfine interactions lie at the origin of their long spin lifetimes [2] but the coupling mechanism of a spin to its environment remains elusive. For instance, spin-phonon coupling, the charges' hopping motion through a disordered local field environment [3], and Elliott-Yafet type spin flips at spatial scattering events [4] can all potentially contribute to spin relaxation.

In this work, we present spin resonance measurements on field induced charges in a transistor architecture down to liquid helium temperatures. We compare coherence and spin lattice relaxation times for a series of state-of-the art donor-acceptor polymers with excellent charge transport properties and demonstrate that spin dynamics at low temperatures are governed by the charge's hopping motion. We identify distinct temperature regimes where competing mechanisms become dominant and show a subtle dependence of spin lifetimes on changes in thin film morphology, corroborated by X-ray scattering and THz vibrational spectroscopy .

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EPR Spectroscopic Signatures of C_{60} and C_{70} Fullerene Cations

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Due to their relatively high reactivity, spectroscopic data are scarce for fullerene cations in condensed matter. Especially EPR parameters seem to depend greatly on the choosen method of cation preparation [1]. Nevertheless, there is a growing interest in charged fullerene species within several research fields. For organic solar cells, the role of cations *vs.* oxidized fullerene derivatives as possible intermediates in charge carrier transport has been discussed [2]. Correspondingly, magnetic resonance methods (EPR, EDMR) rely on precise spectroscopic signatures to identify the different species taking part in such processes. Similarly, potential applications of endohedral group-V fullerenes, either as qubits [3] or as molecular probes for magnetic fields, require identification of competing spin carrying derivatives, namely C_{60} and C_{70} cations or anions.

We therefore used a reported protocol, oxidation of fullerenes via iron(III)-exchanged zeolite NaY, to conduct a systematic study of fullerene cations using EPR spectroscopy at different frequencies (X-, Q-, and W-band).

We correlate our findings with recent EDMR results on fullerene-polymer blend solar cells and N@C_{60}-doped C_{60} microcrystals, highlighting the detection of strongly dipolar-coupled electron spin pairs with possible applications in quantum spintronics.

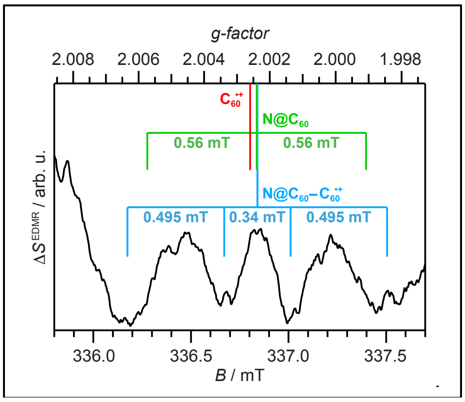

Fig. 1. EDMR difference spectrum of strongly coupled $C_{60}^{\bullet+}$–N@C_{60} [4].

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Poster

Controlling Triplet Excitations by Molecular Design

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Computational methods applied to molecular electronic materials have proved useful both for explaining experimentally observed phenomena, and for the design of new materials with specific properties. When designing molecules for their optical excitation properties, additional design rules can be defined by considering the relationship between the symmetry of the molecule and its excited state properties using group theory. Group theory is a powerful tool to understand spectroscopic properties, explain optical phenomena and define materials' structures in crystals and molecular compounds. The use of group theory to identify eligible families of materials prior to detailed calculation can save time by first identifying any structures that fail some criterion on grounds of symmetry.

Here, we apply group theory and computational methods to design molecules whose lowest energy optical transitions possess some triplet character and are responsive to circularly polarized light. Such structures are of potential interest for organic spintronics. Our procedure is to first identify candidate point groups, then determine the symmetry of excited states using group theory, and then proceed to full calculation of excited states using relativistic quantum chemistry methods. We present preliminary experimental validation of our approach with spectroscopic studies of a new family of molecules.

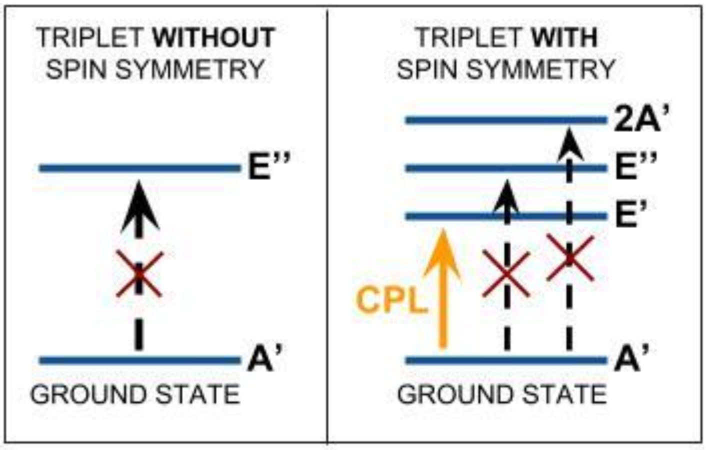

Figure 1: Optically allowed triplet transitions can be predicted using group theory and considering the symmetry of both the excited state and the spin functions. The diagram shows how including spin symmetry affects transitions to the E'' triplet in a molecule with C3h symmetry.

TRESR and EDMR Study of Excitonic and Photocarrier Processes in Vacuum Vapor Deposition Film of Weak Charge Transfer Complex (II)

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We reported the photoconductivity and magnetoconductance effects of the vacuum vapor deposition film of the weak charge-transfer complex (pyrene/dimethylpyromellitdiimid: Py/DMPI) [1]. The magnetoconductance effect of the photocurrent was analyzed by quantum-mechanical simulation assuming two types of collision mechanisms between the electron and hole carriers (DD pair) and between the trapped triplet excitons and mobile carriers (TD pair). A successful simulation was achieved when the parameters (g, D, E, and polarization) determined by Time-Resolved ESR (TRESR) and the effective hyperfine splitting estimated from an ab initio molecular-orbital calculation were used.

In this study, we estimated the depth of the trap for the triplet exciton by measuring the temperature dependence of the single crystal TRESR signal of the charge transfer complex. The single crystal TRESR spectrum was very narrow (the half width of 0.3 mT) at room temperature and the line shape was fitted well with the Lorenz function, indicating mobile exciton with motional narrowing. The signal intensity decreased with the temperature decreasing. The depth of the trap was estimated to be about 1000 K by a fitting with Arrhenius equation assuming a thermally activation. Therefore, many triplet excitons are trapped and the observed species by TRESR is arising from the released one by thermal excitation from the trap. We also measured the electrically detected magnetic resonance (EDMR) of the photocurrent of Py/DMPI vacuum vapor deposition film (Figure 1). The observation of the EDMR signal clarified the existence of weak coupled electron-hole DD pair.

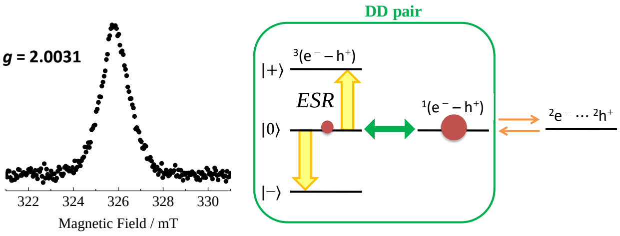

Figure 1: EDMR spectra and Possible Scheme of DD Pair Mechanism in Py/DMPI film.

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Magnetic Field Effects on Photocurrent in Organic Molecular Systems

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The exciton dissociation process in organic systems proceeds *via* a multistep mechanism where the electron-hole pairs (charge transfer states) involved in the current generation process determine the recombination losses and subsequently limit the overall performance of solar cells [1]. Recently, magnetic field effects (MFEs) technique has been recognized as a powerful tool for studying spin-dependent generation and recombination processes of spin-pair species in organic or polymer based solar cells and light emitting diodes [2-5].

In the present work, we focus on the exciton dissociation and charge carriers recombination processes in organic molecular systems based on the studies of the magnetic field effects on photocurrent (magneto-photocurrent, MPC). In organic electron donor:electron acceptor system (m-MTDATA:PBD and m-MTDATA:BCP) the MPC signals are related to the hyperfine interaction modulation and fine structure modulation mechanisms. For squaraine:fullerene solar cells we address the role of electron-hole pair states and charge transfer states in solar cells with various fullerene concentration presenting a detailed photocurrent generation mechanism for both single-layer and bulk-heterojunction solar cells. Depending on temperature and active layer content, the different components operating in the wide magnetic field range contribute to the overall MPC signal [6]. On the other hand, in dye-sensitized solar cells (DSSCs) a crucial role for high photoconversion efficiency play electron transfer processes proceeding at the oxide semiconductor/dye/electrolyte interfaces. We propose a mechanism of photocurrent generation in DSSCs with SQ2, N719 or B1 dye, where the observed MFE is explained by the Δg mechanism [7].

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Recombination Dynamics in P3HT:$PC_{71}BM$ Organic Solar Cell Studied by Magnetoconductance Effect

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Magnetoconductance (MC), which is defined by a change of current density (J) induced by external magnetic field arises from interplay between the spin-selective recombination and the B-field dependent spin conversion of spin pairs, so that the MC effect provides information about the carrier dynamics in organic solar cell under operating condition without destroying device [1]. In order to clarify how the junction structure betwen electron donor (D) and acceptor (A) affects the MC effect, we have measured the MC effects in various types of cells using standard materials of regioregular poly(3-hexylthiophene) (P3HT) as D and [6,6]-phenyl-C_{61}-butyric acid methyl ester $PC_{61}BM$ as A [2]. The results observed for bulk heterojunction cell of P3HT:$PC_{61}BM$ indicate that spin-dependent nongeminate recombination takes place substaintially at the D/A-interface upon illumination of 1 Sun at the short-circuit condition. Although it is well-known that replacement of $PC_{61}BM$ by [6,6]-phenyl-C_{71}-butyric acid methyl ester ($PC_{71}BM$) instead of $PC_{61}BM$ enhances power conversion efficiency because of (i) stronger absorption coefficient and (ii) bicontinuous interpenetrating more crystalline network in active layer [3], no comparative study on the recombination dynamics between P3HT:$PC_{61}BM$ and P3HT:$PC_{71}BM$-cells is reported to the best of our knowledge. Therefore, to elucidate the reccombination dynamics in P3HT:$PC_{71}BM$-cell, we studied on the MC effects under various conditions in this paper. No MC effect due to the nongeminate recombination for the P3HT:$PC_{71}BM$-cell in light were observed within the accuracy of our experiment, although a positive low field MC effect due to the geminate recombination is detected. We will discuss about the spin depedence and efficiency of the recombination on the basis of the light MC effects detected by exciation at different monochromatic wavelengths, transient MC measured using a pulse laser and MC effects in dark.

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Excitons in Topological Molecular Aggregates

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The process of excitonic energy transfer between pigment molecules is widely adopted by phototrophic organisms for the efficient harvesting of solar energy. Understanding of this process is important for the development of organic optoelectronic devices that could be compatible with biological systems and even biodegradable. Recent experiments suggested that excitons in some types of molecular aggregates, which are based on heterotriangulene molecules, propagate on the length scales of several microns at room temperatures [1]. We developed a detailed microscopic model characterizing the transport of excitons in just such structures [2] and applied this model to 2D systems that can be grown experimentally [3]. We show that the exciton bands in 2D aggregates of heterotriagulene pigments can have a non-trivial topology. In analogy to graphene, excitonic Dirac cones are formed near the boundaries of the Brillouin zone in structures with a hexagonal packing, see Fig 1. Moreover, if the molecules are properly functionalized, the cones split resulting in several minima with a non-zero Berry curvature. We suggest that such systems can be used to study topological properties of excitons [4] and also to design photonic devices operating and submicron length scales.

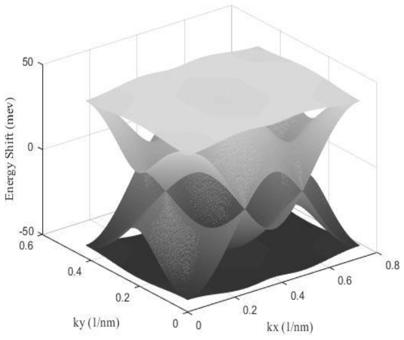

Figure 1 Exciton energy dispersion surface for a hexagonal lattice of heterotrianguelene molecules.

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Oscillating Spin Hall Effect in Organic Chains via Polaron Transport

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Spin Hall effect is a fundamental effect in spin-orbit coupling systems, where a pure spin current along the longitudinal direction is generated by a transverse electric current. In spite of the widely demonstrated Spin Hall effect in metals or semiconductors, the related phenomenon in organic materials are rare due to the weak spin-orbit coupling strength and the completely different transport mechanism. In 2013, Ando et al. experimentally reported an inverse Spin Hall effect in organic materials [1]. Then, a further experiment proved that a spin current can be carried by polarons in organic semiconductor [2]. The latter work indicates the importance of polarons in such novel spin-orbit effects in organic materials. Although a theoretical investigation of Spin Hall effect in disordered organic solids have been performed by Yu [3], a direct simulation of polaron transport in organic materials is still lack.

In this work, based on an extended Su-Schrieffer-Heeger (SSH) model with a Rashba spin-orbit coupling term, the polaron transport in 2D polymer chains is simulated with nonadiabatic dynamic method. The results demonstrate that a preexisting polaron located in the central chain may transport both in the transverse direction along the chain and in the longitudinal direction between chains. For a spin degenerated initial state, the longitudinal hopping of the polaron induces a pure spin density perpendicular to the transverse electric current. The net spins in the two side chains oscillate between positive and negative values, which indicates an oscillating Spin Hall effect. The frequency of the oscillation is discussed.

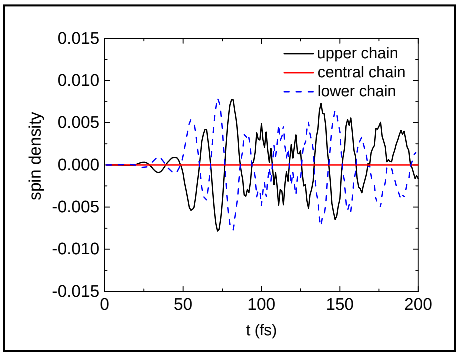

Figure 1: Evolution of spin density with time for a mixed polaron initially located in the central chain.

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Magnetic Field Effect on Pentacene-Doped Sexithiophene Diodes

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Magnetic field effects observed in various organic devices are of great scientific interest because of their large magnetoresistance (MR) up to 10% at room temperature and under small magnetic fields of approximately 10 mT without ferromagnetic contacts [1]. In this work, we studied the effect of impurities on the magnetoresistance of sexithiophene-based diodes using impedance spectroscopy. The impurities were introduced by doping pentacene molecules into a sexithiophene film through a co-evaporation process. The pentacene molecules act as charge-scattering centers, which trigger the negative magnetoresistance of the device. This makes it possible to tune the value of magnetoresistance from positive to negative by increasing the applied voltage. The beneficial properties induced by impurities suggest a potential route to integrate additional functions into organic devices.

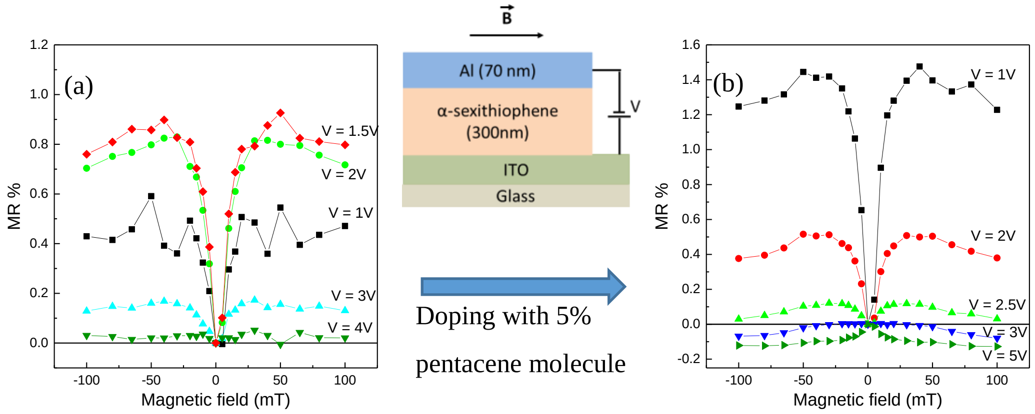

Figure 1: Effect of traps on ITO/sexithiophene/Al device: (a) the device showed only positive MR and (b) the device with doping 5% pentacene showed larger positive MR, and a small negative MR appeared.

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MAGNETORESISTANCE IN ORGANIC SPIN-VALVE AT ROOM TEMPERATURE

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Abstract

Organic spintronics is an exciting new research area, as it combines electron polarised spin transport with organic semiconductors. The research work focuses on the development of organic based spintronic devices consisting of magnetic/Organic semiconductor (spacer)/magnetic trilayers [1, 2]. The long spin coherence due to the weak spin orbit interaction in organic materials makes them more suitable for spintronic devices. Magnetoresistance (MR) measurements were carried out by applying a current perpendicular to the film plane with the field parallel to the film plane. At room temperature we studied the magnetoresistance of organic spin-valves using Rubrene ($C_{42}H_{28}$) as the spacer layer. The choice of the electrode material is important for spin injection. The work function of FeCo (4.7eV) and NiFe (4.5eV) are close to the HOMO energy (5.4eV) of Rubrene, thus the device showed ohmic behavior. For the spin-valve effect the two ferromagnetic electrodes should have different coercive fields for independent switching by applying a magnetic field. The $Fe_{70}Co_{30}$ which has harder magnetic properties was chosen as the bottom electrode and the top electrode was $Ni_{80}Fe_{20}$ which has very soft magnetic properties. The Fig 1 shows the normalized VSM magnetization loop which confirms the spin-valve effect. The MR was measured as a function of Rubrene thickness. At thicknesses 120nm, the MR was ~0.3% at room temperature.

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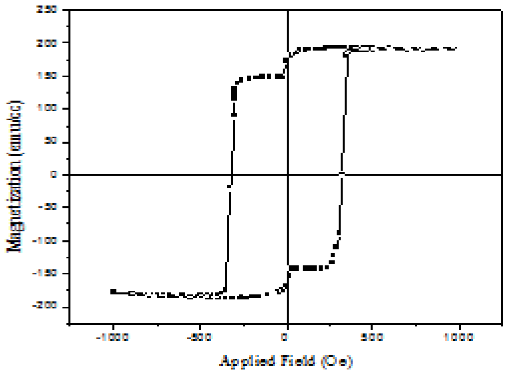

Figure 1: The magnetic hysteresis loop on top of the organic spin valve stack.

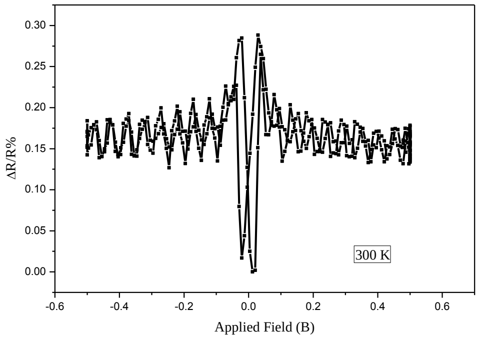

Figure 2: MR of the organic spin valve device

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Light induced magnetoresistance in solution processed planar hybrid devices measured under ambient conditions

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We report light induced negative organic magnetoresistance (OMAR) measured under ambient atmosphere in solution processed 6,13-bis(triisopropylsilylethynyl)-pentacene (TIPS-pentacene) planar hybrid devices of two different device architectures. Hybrid electronic devices with trench isolated electrodes (HED-TIE) having channel length of ~100 nm fabricated in this work and, for comparison, commercially available pre-structured organic field effect transistor (OFET) substrates with channel length of 20 μm were used. The magnitude of the photocurrent as well as the magnetoresistance was found to be higher for the HED-TIE devices due to much smaller (~100 nm) channel length of these devices compared to the OFETs (20 μm). We attribute the observed light induced negative magnetoresistance in TIPS-pentacene to the presence of electron-hole pairs under illumination as the magnetoresistive effect scales with the photocurrent [1]. The magnetoresistance effect was found to diminish over time under ambient conditions compared to a freshly prepared sample. We propose that the much faster degradation of the magnetoresistance effect as compared to the photocurrent was due to the incorporation of water molecules in the TIPS-pentacene film [1].

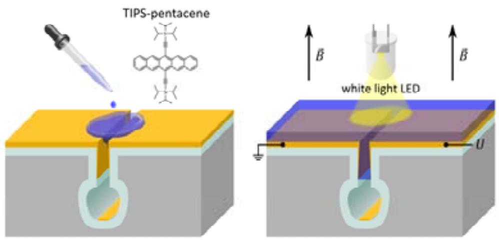

Figure 1: Sketch of the experiments

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Magneto-conductance and Magneto-electroluminescence in High Magnetic Field in Organic Light Emitting Diodes

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We have investigated magnetic field effects in low and high fields (B, up to 8 Tesla with high resolution of ~10^{-4} Tesla at low fields) over the temperature range 280-30 K in light emitting diodes made up of P3HT and super yellow (SY) organic semiconductors. In these devices we have measured magneto-conductance (MC), and magneto-electroluminescence (MEL). At 280 K we find that the MC(B) and MEL(B) responses are identical (up to a B independent constant) and show near-saturation above B~2 T indicating that they are caused by identical species. However, at low temperatures they show different field dependent responses pointing toward the possibility of additional species that contribute to MEL(B).

In these low mobility substances magnetic field effects are attributed to the spin degrees of freedom. We explain the MC and MEL experimental results by studying the effect of magnetic field on polaron pairs composed of oppositely charged species with spin 1/2. In the low field regime (~10mT) the magnetic field effects are caused by the hyperfine interaction between the spins of the polarons and the spins of the many protons that are present in all organic substances. In the intermediate field regime we consider a mechanism that was not discussed in detail previously and is caused by the anisotropy of the g-factor in these low symmetry organic molecules. The anisotropic g-tensor makes the levels containing the singlet S and triplet T_0 spin configurations vary with magnetic field, similar to the well-known Δg mechanism in devices where the positive and negative charges are on different molecules. In high fields (higher than 2 Tesla) we consider partial thermal spin polarization as an additional mechanism contributing to the magneto-effects. We have developed a simplified quantum mechanical approach taking into account the hyperfine and exchange interactions together with g-anisotropy and thermal effects. With this model we could account for the observed experimental data and draw conclusions about the exchange interaction between polarons that compose the polaron pair, the orientation of the g-tensors within the polaron pair in organic semiconductor and about the life time of polaron pairs in these organic light emitting diodes.

TMR in Magnetic Tunnel Junctions with Phenalenyl-molecule Tunnel Barriers

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Phenalenyl (PLY) based molecules, which can be regarded as Graphene fragments are promising candidates for spintronic applications. Attempts to use open shell PLY molecules have been unsuccessful due to their instability. We investigated a new closed shell molecule, PLY with a Copper complex, for its spintronics suitability. TMR in various samples of PLY-Cu MTJ's was determined by measuring the resistance across the MTJ under a high magnetic field during parallel and anti-parallel configurations of the ferromagnets (FMs). Preliminary results show outstanding Magnetoresistance (MR) at room temperature. Our works demonstrate convincingly that spin-polarized currents can be injected into organic materials with reasonably high efficiency, providing strong evidence of spin polarized tunneling as the dominant transport mechanism in PLY-Cu based magnetic tunnel junctions, and the use of PLY-based molecules as a viable and scalable platform for building molecular-scale quantum spin memory and processors for technological development.

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Spontaneous spin polarization of methanol molecule adsorbed on B- or N-doped graphene: first-principles calculations

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Graphene based all organic spintronic devices attracted people's research interest in spintronics[1-3]. The spontaneous spin polarization properties of methanol molecule adsorbed on the graphene surface with boron and nitrogen atoms are studied by first principles calculations. It can be obtained that the methanol molecule could be spin polarized even there is no magnetic elements in the whole systems. The densities of states of the molecule are spin nondegenerate near the Fermi level after the adsorption. The p-orbital couplings between the methanol molecule and the graphene generate new spin coupling states, and the transferred charge from the graphene to the molecule will fill these spin nondegenerate states, which leads to obvious spontaneous spin polarization of the methanol molecule. The spin density distributions, differential charge density distributions as well as the charge transfer of the systems also suggest that the spin polarization of the methanol molecule will be the biggest one when it is adsorbed on the top site of the graphene surface with N acting as anchor. Our calculations can contribute to the studies of spontaneous spin polarization in graphene based all organic spintronic devices.

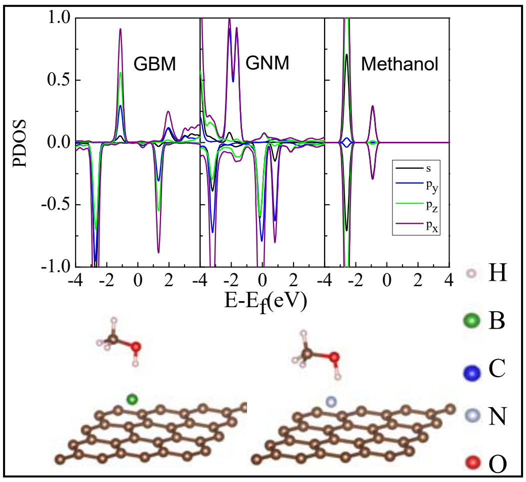

Figure 1: Projected density of states for methanol molecule adsorbed on graphene surface with B or N as anchors.

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EPR Study of Spin Dependent Charge Transfer Processes at Functionalized Electrodes

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We want to look for a spin-dependence in the charge transfer that occurs at the interface between an electrode and an electrolyte. Chazalviel found evidence for spin-dependence of the electron transfer on Methyl Viologen (MV) [1]. However, magneto-hydrodynamic effects may have played a role since he used a very large field range, from -2.5 to +2.5 T [2]. To avoid this spurious effect, we use electrically detected electron paramagnetic resonance (ED-EPR) to detect a spin effect without changing the field significantly.

We have developed an oxygen-tight electrochemical cell with different working electrodes, a silver wire reference electrode and a platinum wire counter electrode, in a geometry compatible with EPR measurements. $MV^{+\cdot}$ radicals are produced either electrochemically ex-situ or in situ with a Pt wire as sacrificial working electrode. For the working electrode, we are using p-GaAs and GaN/AlGaN functionalized with chiral molecules [3]. Cyclic voltammograms and impedance measurements around the two reduction potentials of MV are performed. We measure simultaneously the standard continuous wave EPR (9.8 GHz) signal and the cell current and its modulation. For various fields around the resonance condition, we measure the cell current while scanning the working electrode potential through both MV reduction peaks. With lock-in technique we monitor sample-orientation dependent spin resonance for the potential modulated current of the cell when the working electrode is functionalized with chiral-molecules. This result is consistent with other recent observations when the GaN/AlGaN electrodes were used [4].

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Ferroelectric control of organic/ferromagnetic spinterface

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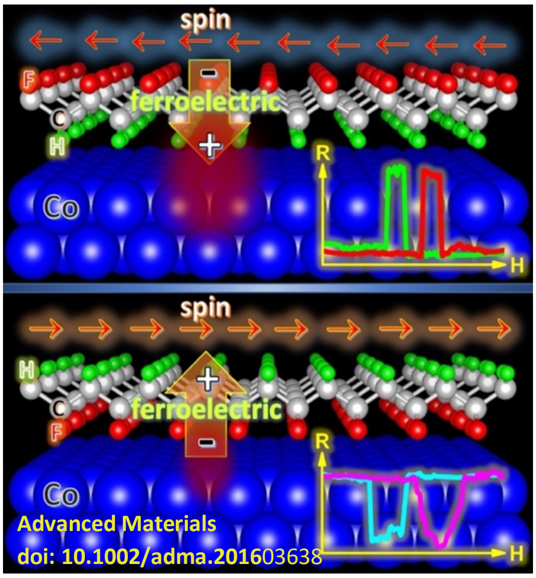
Hybrid ferromagnetic metal/organic interface, as known as "spinterface", can exhibit highly efficient spin-filtering properties and therefore present a promising class of materials for future spintronic devices. The spin-polarization of spinterface at Fermi level can be different or even opposite in sign to that of adjacent ferromagnetic electrode. To achieve desired injection of spin-polarization, one should carefully engineer the organic/ferromagnetic interface to precisely tailor their electronic properties. Here, by using ferroelectric organic material poly(vinylidene fluoride) (PVDF), we demonstrate that the spin-polarization of the PVDF/Co spinterface can be actively controlled by tuning the ferroelectric polarization of PVDF [1]. In particular, we have fabricated organic multiferroic tunnel junctions (MFTJs) based on La$_{0.6}$Sr$_{0.4}$MnO$_3$/PVDF/Co structures. The tunneling magnetoresistance (TMR) sign can be changed by electrically switching the ferroelectric polarization of PVDF barrier. This study opens new functionality in controlling the injection of spin polarization into organic materials via the ferroelectric polarization of the barrier.



Advanced Materials
doi: 10.1002/adma.201603638

Figure 1: Ferroelectric control polarization of PVDF to modify spin-polarization at PVDF/Co « spinterface ».

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Substitution effect on electronic and magnetic properties of double perovskite Sr_2FeMoO_6

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Transition metal oxides constitute a large class of materials with variety of very interesting properties and important technological utility. A subset with double perovskite structure doped Lanthanides has been the subject matter of the current theoretical investigation with an emphasis on their electronic and magnetic behavior. The aim of this study is to calculate the electronic, and magnetic properties for Sr_2FeMoO_6, doped La, Nb, and Y. The first principles calculations are carried out using the density functional theory formalism as implemented in Wien2K code.

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Easy-plane ferroborates. Magnetopiezoelectric effects

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Rare-earth borates with formula $RFe_3(BO_3)_4$ (R = Y; La-Nd; Sm-Er) are popular object of study because they the materials which combine magnetically ordered and ferroelectric media properties. This is why ferroborates belong to the family of multiferroics[1].

Since ferroborates belong to noncentrosymmetric class 32, the direct piezoelectric effect (PE) is allowed in these crystals. We have investigated the piezoelectric properties of $SmFe_3(BO_3)_4$ and $NdFe_3(BO_3)_4$ single crystals using the acoustic method [2]. It was found that in those compounds, the value of the piezoelectric modulus e11 in the paraelectric phase (≈ 1.4 C/m^2) was almost an order of magnitude higher than that of the α - quartz, and, therefore, such compounds may be recommended for technical applications.

In addition to the above-mentioned direct PE in multiferroics the indirect PE may exist. It consists in the joint action of the magnetoelastic and magnetoelectric mechanisms. Due to magnetoelasticity deformation changes the state of magnetic variables and through the magnetoelectric coupling excites the electric field (and vice versa). This effect was first discovered in samarium ferroborate [3].

In $NdFe_3(BO_3)_4$ direct renormalization of the piezoelectric interaction in a magnetically ordered phase is observed [4].

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Half-Metallic Completely Compensated Ferrimagnets in Cr doped BaP

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On the basis of ab-initio calculations we have investigated the electronic and magnetic properties of Cr1-xBaxP alloy, our calculations suggest that as we dope BaP with Cr atoms and move towards Cr1-xBaxP where x=0, 0.125, 0.25, 0.50, and 0.75 all alloy are HM-FM. Interestingly Cr0.25Ba0.75P is a HM-AFM otherwise 'fully compensated ferrimagnet', this alloy should be of special interest for applications since it creates no external stray field and thus exhibit minimal energy losses. In addition, the robustness of half-metallicity with respect to the variation of lattice constants of Cr1-xBaxP is also discussed; Moreover ferrimagnetism co-exists with the half-metallicity, resulting in the desired fully compensated half-metallic ferrimagnetism, for a wide range of lattice constants. Furthermore we found that this new HMFCF is stable according to its small formation energy. First

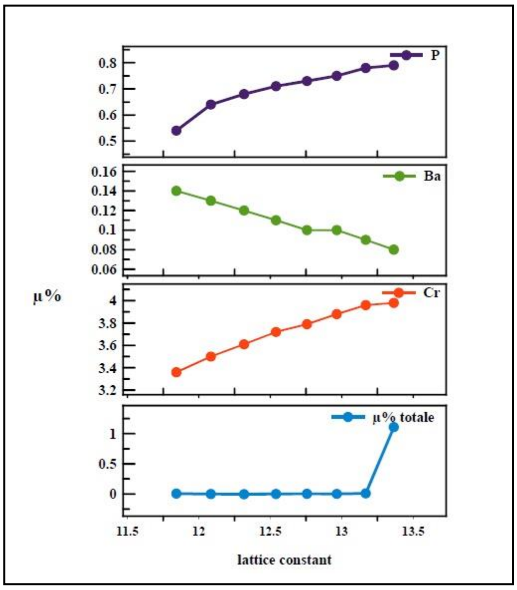

Figure 1: The total magnetic moment, the magnetic moments of the atoms, and the polarization of spin according to the constant lattice

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Interlayer Exchange Coupling between Ferromagnetic Films through Topological Insulators

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Spintronics Is The Branch Of Physics For The Study Of The Intrinsic Feature Of The Electron (spin), And Its Associated Magnetic Moment, In Addition To Its Fundamental Electronic Charge In Solid State Devices. Spintronics Emerged From In The 1980s Concerning Spin-Dependent Electron Transport Phenomena In Solid-State Devices. This Includes The Discovery Of Giant Magnetoresistive (gmr) Independently By Albert Fert And Peter Grunberg (1988). The Most Straightforward Giant Magnetoresistive Device Contains A Paramagnetic Layer Which Is Sandwiched By Ferromagnetic Films. The Study Of These Structures Has Been Done For Both Metallic And Insulators Spacer. The Topological Insulators Are A New Phase Of Matter That Has Noticeable Features Like Spin-Momentum Locking. These Substances Are Conductance In The Surface And Insulator-Like In Bulk.

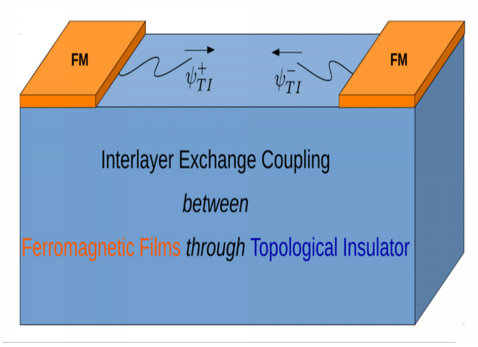

Figure 1: Schematic of ferromagnetic films which put on the bulk topological insulator .

We Investigated The Interlayer Exchange Coupling (IEC) Between Ferromagnetic Films Through Topological Insulators. This Study Has Been Done In Terms Of Quantum Interferences Due To Confinement Of Electron Wave Function. This Approach Provides A Remarkable Physical View Of The Interlayer Exchange Coupling Mechanism. In This Thesis, We Found That The Interlayer Exchange Coupling Between Ferromagnetic Films Is Independent Of Magnetism In The X-Direction. Moreover, It Is Different For Various Ferromagnetism Configurations.

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Low Temperature Reflux Synthesis and Study of Cobalt Ferrite Nanoparticles

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The magnetic nano-particles have aroused widespread interest due to their exceptional magnetic properties and unique applications. Among these magnetic nano-particles, cobalt spinel ferrite, has gained prominence due to its high coercivity (Hc), moderate saturation magnetization (Ms), good chemical stability and high mechanical hardness [1]. These properties make it a promising material for high-density magnetic recording, permanent magnets, magnetic fluids, catalysis and photo-magnetic material [2].

In the present work, cobalt ferrite nanoparticles were synthesized using reflux method. X-ray Diffraction (XRD) pattern as shown in figure 1(a) shows the single phase nature with cubic crystal structure and matches well with standard JCPDS data (card no. 01-077-0426). The average particle size ~6 nm was estimated from the Transmission Electron Microscope (TEM) (figure 1(b)). A SQUID-VSM magnetometer was utilized to study the magnetic properties of $CoFe_2O_4$ nanoparticles. The $CoFe_2O_4$ nanoparticles shows the ferromagnetic nature both at room temperature (300 K) and low temperature (70 k). The chemical, elemental and structural/compositional information was analyzed using X-ray photoelectron spectroscopy (XPS). Valance Band Spectra (VBS) for cobalt ferrite at different incident photon energies is carried out to study the nature of valance band. The work function for $CoFe_2O_4$ nanoparticles is also calculated using these VBS (figure 1(c)) and it is found to be ~ 4.9 eV.

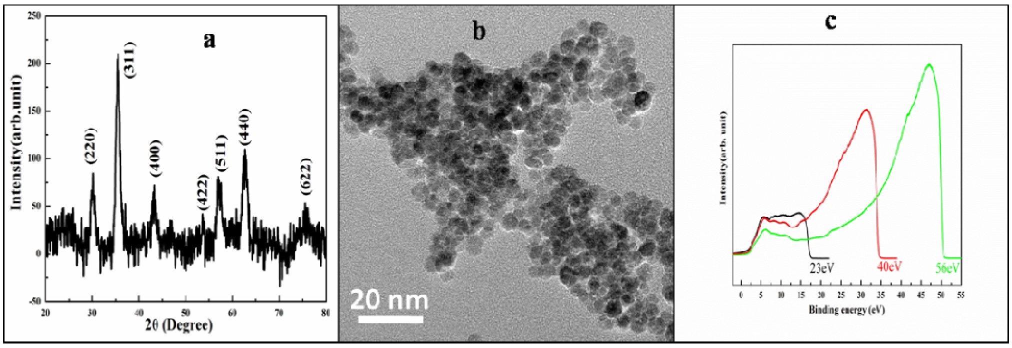

Figure 1: (a) XRD pattern, (b) TEM image and (c) VBS spectra of $CoFe_2O_4$ nanoparticles

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Half metallic Fe_3O_4 thin films for organic spintronic

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Investigation of Fe_3O_4 [$(Fe^{+3})^A(Fe^{+2},Fe^{+3})^BO_4$] thin films continue to be an avenue for organic spintronic. Electron hoping between Fe^{+2} and Fe^{+3} ions at tetrahedral B-sites of Fe_3O_4 facilities room temperature electric conductivity $\sigma = 200\ (\Omega\text{-cm})^{-1}$ (about 0.1% of Cu metal) in Fe_3O_4 if otherwise ferrites are mostly insulators. On the top of this; Fe_3O_4 owns only one type of spin band (d orbit electron –ve spin t_{2g}) at Fermi level, demonstrating half metallic character which has triggered many spin polarization based applications [1]. Herein, nanocrystalline Fe_3O_4 thin films were synthesized by adopting two different reduction approaches (1) vacuum annealing and (2) wet H_2 annealing. While vacuum annealed films shows Verwey transition with lower resistivity compared to the bulk Fe_3O_4, the same was not observed in electric transport properties of wet H_2 annealed films. However, this transition was clearly seen in the temperature dependence of magnetizations of both sets of Fe_3O_4 thin films. This seems to indicate that both the electric transport and magnetization are two independent processes; it's just coincidence to happen at same place of Verwey transition at 120 K. Different electric transport properties in both reductions treated Fe_3O_4 films could be ascribed to different grain sizes/grain boundary volumes, inhomogeneities and presence of residual atomic-H at grain boundaries emanating from complex reductions treatments.

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Observation of Dzyaloshinskii-Moriya interaction in Co/Pt multilayers

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Dzyaloshinskii-Moriya interaction (DMI) has been known to play an important role in both field- or current-driven magnetic domain wall motions[1]. The DMI takes part in forming a Néel-type domain wall (DW) in magnetic films[2], where magnetic field causes the transformation the wall type from the Bloch into the Néel one by the broken inversion symmetry at the interface. In this work, we report our observation of DMI in Co/Pt multilayers with variation of Co sublayer thickness and multilayer repeat numbers. The domain evolution patterns under fields were investigated by means of a magneto-optical Kerr effect microscopy, where asymmetric DW extension was immediately observable. The DW velocity under out-of-plane fields can be described by the creep law, which can be expressed by the power law behavior with a conventional creep critical exponent. Effective DMI constant is extracted by using the relation, $D = \mu_0 H_{DMI} M_S \Delta$. The magnetization within DWs is observed to be no longer pointed from black to white domains under longitudinal magnetic field, implying a transformation from a left-hand to a right-handed Néel wall. Interface effect between the Ta and the Co/Pt multilayer is also discussed.

This research has been supported by [Grant No 2015R1D1A3A01020686] and by Max Planck POSTECH/KOREA Research Initiative Program [Grant No 2016K1A4A4A01922028] through the National Research Foundation of Korea (NRF).

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Integration of Molecular Quantum Bits with Organic Semiconductor Spintronics

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Molecular nanomagnets hold great promise for quantum computing, as they have been shown to exhibit coherence times from tens of microseconds up to almost a millisecond [1]. The molecular nature of these systems offers the possibility for extended chemical tailoring for higher coherence times or surface self-assembly [2].

However, local addresing of molecular qubits is very challenging and for succesfull device development, these qubits will need to be interfaced with inorganic and/or organic semicondutor technology. To overcome this challenge, we plan to use (spin polarized) charge carriers with various possibilities to programme/readout of the quantum state of the qubits.

To investigate the possibility of interfacing magnetic molecules with organic semiconductor technology, we are manufacturing hybrid materials made of conducting polymers and molecular qubits. We have successfully observed quantum coherence in the microsecond regime in thin films of these hybrid materials using a custom Fabry-Pérot resonator at 35 GHz. In the next step, we want to study the interaction between mobile charge carriers and localized magnetic moments using electrically detected magnetic resonance.

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Study of 12-Metallacrowns-4 Complexes

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After the first observation of the slow magnetization relaxation below the blocking temperature of the Mn(III)/(IV) ion containing Mn12 cluster [1], single molecular magnets (SMM) are also considered as building blocks for spintronic devices. Because SMMs decompose in ultra-high vacuum, one usually prepares ultrathin, substrate-supported SMM layers with a solvent-based procedure.

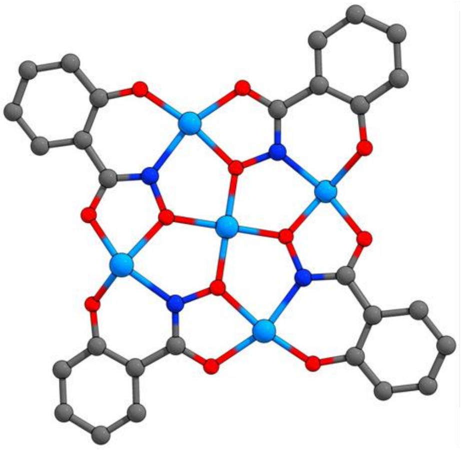

Figure 1: $(HNEt_3)_2[CuCu_4(shi)_4]$, with a homogeneous- Cu-core

Here, we present $(HNEt_3)_2[CuCu_4(shi)_4]$, (Fig.1) with only Cu metal ions, and the heterogeneous-core structure $(OCH_2NMe_2)_6[CuFe_4(shi)_4]Cl_2$ [3]. We utilize different film preparation techniques (from an *ex situ* nonisotropic solvent evaporation casting technique to *in situ* ultrahigh vacuum e-spray deposition). X-ray photoelectron spectroscopy shows that different layer thicknesses, deposited on different substrates, can be prepared avoiding homo- and heterolytic cleavage of the metal core frame.

Using state-of-the-art quantum-chemistry we calculate all lowest electronic states with various multiplicities, and we show that due to the interplay of more subtle mechanisms (e.g., multicenter Coulomb integrals), it is necessary to go beyond the Goodenough-Kanamori rules to determine the sign of the exchange coupling constants [3]. Finally, measuring the experimental electronic spectra of the valence electrons of both complexes in thin layers containing only molecules, which are not effected by any kind of interface interaction, we compare these molecular states with the theoretical ones.

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8:40	Opening remarks			
8:50		I 6 - Reineke	I 9 - Sirringhaus	I 11 - Kawakami
9:00	I 1 - Gruber			
9:10				
9:20		O 10 - Chepelianskii	O 25 - Qaid	O 31 - Moorsom
9:30	I 2 - Bürgler			
9:40		O 11 - Meyer	O 26 - Wittmann	O 32 - Morawetz
9:50				
10:00	I 3 - Ardavan	O 12 - Drew	O 27 - Cox	O 33 - Rogers
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10:20		Coffee break/Posters	Coffee break/Posters	Coffee break
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10:40		I 7 - Zhu	I 10 - Richter	I 12 - Boehme
10:50	O 1 - van Slageren			
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11:10	O 2 - Buks	O 13 - Teki	O 28 - Mahani	O 34 - Yang
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11:30	O 3 - Riminucci	O 14 - Johnston Halperin	O 29 - Nicolaides	O 35 - Schott
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12:10			Free time	Closing remarks
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