Dresden 2017 – TT Tuesday

## TT 34: Spintronics, incl. Quantum Dynamics (joint session DS, HL, MA, TT, organized by MA)

Time: Tuesday 14:00–15:45 Location: HSZ 301

TT 34.1 Tue 14:00 HSZ 301

Prediction of an intrinsic spin Hall effect without spin-orbit coupling in non-collinear antiferromagnets — •Yang Zhang<sup>1,2</sup>, Jakub Zelezny<sup>1</sup>, Jeroen van den Brink<sup>2</sup>, Claudia Felser<sup>1</sup>, and Binghai Yan<sup>1,3</sup> — ¹Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — ²Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — ³Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The spin Hall effect (SHE), which converts a charge current into a transverse spin current, has long been believed to be a phenomenon induced by the spin-orbit coupling. In this work, we have revealed the existence of an intrinsic SHE without the spin-orbit coupling by theoretical calculations. Such a SHE is realised in the chiral spin structure of non-collinear antiferromagnets, even when the scalar spin chirality is zero. We have obtained large intrinsic spin Hall conductivity in related compounds Mn 3 Ge and Mn 3 Sn, that are chiral antiferromagnetic above room temperature and also predicted to be Weyl semimetals recently. Our work provides further understanding on the spin Hall effect and paves a new way to design SHE materials based on the chiral magnetic materials.

TT 34.2 Tue 14:15 HSZ 301

Ising spintronics in transition-metal dichalcognides — •BIN SHAO¹, MALTE SCHÜLER¹,², GUNNAR SCHÖNHOFF¹,², THOMAS FRAUENHEIM¹, GERD CZYCHOLL², and TIM WEHLING¹,² — ¹Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany — ²Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

The orbital character of charge carriers at the Fermi level of transition-metal dichalcognides,  $MX_2$  ( $M=\mathrm{Mo}$ , W;  $X=\mathrm{S}$ , Se, Te), can be selected via doping levels, leading to orbital dependent spin-flip scatterings with magnetic adatoms on  $MX_2$ . By utilizing this feature, we propose a mechanism for Ising spintronics relying on the tunability of spin lifetime of transition-metal adatoms with  $d^9$  configuration on a  $MX_2$  monolayer. The spin lifetime can be tuned by more than two orders by shifting the Fermi level only slightly. Moreover, the system exhibits a sizable magnetic anisotropy. We calculate the spin lifetime and magnetic anisotropy of magnetic adatoms based on an effective model Hamiltonian, reveling their connections to doping levels and the symmetry of adsorption sites straightforwardly. Our ab initio calculations suggest that this Ising-type spintronics should be realizable in Co, Rh, or Ir adatoms on  $\mathrm{MoS}_2$ .

TT 34.3 Tue 14:30 HSZ 301

A three-input majority gate with chiral magnetic solitons — Konstantinos Koumpouras<sup>1</sup>, Dmitry Yudin<sup>2</sup>, Danny Thonig<sup>1</sup>, Christoph Adelmann<sup>3</sup>, Anders Bergman<sup>1</sup>, Olle Eriksson<sup>1</sup>, and •Manuel Pereiro<sup>1</sup> — <sup>1</sup>Department of Physics and Astronomy, University Uppsala, Sweden — <sup>2</sup>ITMO University, Saint Petersburg 197101, Russia — <sup>3</sup>IMEC vzw. Kapeldreef 75, B-3001 Leuven, Belgium

In magnetic materials, nontrivial spin textures may emerge owing to the competition among different types of magnetic interactions. In particular, chiral magnetic solitons, represent topologically protected spin configuration with particle-like properties, that are ideally suited to perform logical operations. Based on atomistic spin dynamics simulations, we propose to make use of magnetic solitons in a functional and dynamic three-input majority gate, in which the input states can be controlled by applying an external electromagnetic field or spin-polarized currents. One of the main advantages of the proposed device is that the input and output signals are encoded in the chirality of solitons, allowing to perform logical operations. As examples we illustrate how the proposed device can be used to perform logical relations such as Boolean AND and OR.

TT 34.4 Tue 14:45 HSZ 301

Spin-torque Effects in Thermally Assisted Magnetization Reversal: Kramers' Escape Rate Theory Approach — Yuri P. Kalmykov<sup>1</sup>, Declan J. Byrne<sup>2</sup>, •William T. Coffey<sup>3</sup>, William J. Dowling<sup>3</sup>, Sergey V. Titov<sup>4</sup>, and Jean Eric Wegrowe<sup>5</sup> —

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Thermal fluctuations of nanomagnets driven by spin-polarized currents are treated via the Landau-Lifshitz-Gilbert equation generalized to include both the random thermal noise field and the Slonczewski spin-transfer torque (STT) term. The reversal time of the magnetization in such a nanomagnet are evaluated for wide ranges of damping by using the method of Coffey et al. [Phys. Rev. E 63, 021102 (2001)]. Their method generalizes the Mel'nikov-Meshkov approach [J. Chem. Phys. 85, 1018 (1986)] for bridging the very low damping (VLD) and intermediate damping (ID) Kramers escape rates for mechanical Brownian particles (the Kramers turnover problem) to the analogous magnetic turnover problem.

TT 34.5 Tue 15:00 HSZ 301

Inducing spin in semiconducting 2D phosphorene — •Mukul Kabir — Department of Physics, and Centre for Energy Science, Indian Institute of Science Education and Research, Pune, India

Inducing magnetic moment in otherwise nonmagnetic two-dimensional semiconducting materials is the key first step to design spintronic materials. In this talk, we will address the feasibility of inducing such local moment in single-layer phosphorene through 3d transition-metal (TM) doping without affecting its intrinsic semiconducting nature. While adjudicating on this subject, all previous studies conveniently neglected TM diffusion. However, we predict that increased TM diffusivity on pristine phosphorene would severely hinder any possibility of controlled magnetism, and thus any application. Here we propose that the pointdefects will anchor metals, and exponentially reduce the diffusivity. We further argue that the divacancy complex is imperative in any practical purpose due to their increased thermodynamic stability over monovacancy. For most cases, the defect-transition metal complexes retain the intrinsic semiconducting properties, and also induce a local magnetic moment with large exchange-splitting and spin-flip energies, which are necessary for spintronic applications. Further, we provide a simple microscopic model to describe the local moment formation in these transition metal and defect complexes. Moreover, such metal absorption could completely alter the intrinsic electronic structure of the single-layer phosphorene, and may lead to exotic many-body physics.

TT 34.6 Tue 15:15 HSZ 301

Adsorption and element-specific detection of transition metal porphyrins by spin-dependent conductance of a graphene nanoribbon — •Peter Kratzer<sup>1</sup>, Sherif A. Tawfik<sup>2</sup>, Xiang Yuan Cui<sup>2</sup>, and Catherine Stampfl<sup>2</sup> — <sup>1</sup>Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — <sup>2</sup>The University of Sydney, Sydney, New South Wales 2006, Australia

Transition metal porphyrins, their adsorption on graphene nanoribbons (GNRs), and its consequences for electronic transport through the GNRs are investigated by means of density functional theory calculations. Interaction with a single-atom vacancy in the GNR is found to be a prerequisite for chemical bonding of the transition metal centre. In both the physisorbed and the chemisorbed geometry, the inclusion of van der Waals interaction results in a significant enlargement of the binding energy. Electronic transport calculations using nonequilibrium Greens functions show that the conductivity of the edge states in the GNR is altered by the chemisorbed porphyrin molecules. Since the metal centers of porphyrins carry an element-specific magnetic moment, the spin-dependence of the conductance of the GNR is altered, too. In particular, the adsorption of Ru-porphyrin or Feporphyrin on the single-atom vacancy results in a large spin polarization of the current of 88% and -62%, respectively, at small applied source-drain voltages. Based on our results, we suggest that a spin valve constructed from a GNR with ferromagnetic contacts could be used as a sensitive detector that could discriminate between various metal porphyrins.

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TT 34.7 Tue 15:30 HSZ 301

Shape Memory Alloys in Hybrid Spintronic Devices — • Andreas Becker and Andreas Hütten — Bielefeld University, Bielefeld, Germany

Observations of the phase transition in ferromagnetic shape memory alloys (FSMAs) by x-ray diffraction and magnetization measurements are reported frequently. Our goal is to investigate the phase transformation by using the tunnel magnetoresistance effect (TMR), thus FSMAs are utilized either as ferromagnetic electrodes (Ni50-xCoxMn30Al20/MgO/ Co40Fe40B20) or as an underlying layer beneath the magnetic tunnel junction (Ni50-xCoxMn30Al20/Co40Fe40B20/MgO/ Co40Fe40B20).

The off-stoichiometric Ni50-xCoxMn30Al20 thin films are grown by sputter deposition and patterned by e-beam lithography. X-ray diffraction measurements indicate a B2 crystal structure. An untypical change in the TMR amplitude is observed in tunnel junctions on top of the Heusler alloy upon heating the sample. We suggest that this phenomenon arises from the induced strain of the reverse martensitic transformation. Furthermore the FSMA will act as a ferromagnetic electrode if the magnetic properties are enhanced by substituting Ni with Co atoms. At x=10 a TMR of about 2.5% at room temperature and 6% at 10 K is measured in Ni50-xCoxMn30Al20 /MgO/Co40Fe40B20 tunnel junctions while no TMR is found over the measured temperature range in samples with x=4.