

MA 36: Spin-Dependent 2D Phenomena

Time: Wednesday 15:00–18:00

Location: HSZ 101

Invited Talk

MA 36.1 Wed 15:00 HSZ 101

2D Magnetic Materials — ●ALBERTO MORPURGO — University of Geneva, Geneva, Switzerland

The first 2D magnetic material in which ferromagnetism has been shown experimentally to persist down to individual monolayers has been reported less than two years ago. Since then a number of different experiments have been performed on atomically thin magnets of different types, and led to interesting observations (giant tunneling magneto resistance, gate-tuning of the magnetic state, strong exchange bias at van der Waals interfaces, etc.). In my talk I will give a short introduction to this rapidly evolving domain of research, and discuss results obtained in my group on atomically thin multilayers of materials such as CrI₃, CrCl₃ (layered antiferromagnets) and MnPS₃ (antiferromagnetic within individual layers). Most of our experiments focus on investigations of the magnetic properties of atomically thin crystals of these materials by using them to form tunnel barriers and by measuring their tunneling magnetoresistance. As I will show, tunneling magnetoresistance allows tracing the boundaries between different magnetic phases, and it can therefore be used to establish magnetic phase diagrams. Specific phenomena that I will discuss include the observation of a giant tunneling magnetoresistance in CrI₃, a complete analysis of the magnetic phases of multilayers of CrCl₃ as a function of thickness, magnetic field and temperature, and the observation of a spin-flop transition in MnPS₃ persisting to the ultimate thickness of an individual monolayer.

MA 36.2 Wed 15:30 HSZ 101

Strain-induced phase transition in CrI₃ bilayers — ●ANDREA LEON — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Recent reports on ferromagnetic and antiferromagnetic order in different 2D crystal Van der Waals heterostructures, have opened a vast field of possibilities for new physical phenomena and generation of electronic devices which already started to be explored experimentally. In particular layered CrI₃ systems are of great interest due to the staking dependent magnetism, mechanical/magnetic response under pressure, magnetoelectric and optical properties, between others. Motivated by this, the main goal of this work is to search for new electronic properties of antiferromagnetically coupled CrI₃ bilayer with C₂/m symmetry under strain, using DFT calculations and analytic models. We found that strain may be an efficient tool to tune the magnetic phase of the structure. A tensile strain stabilizes the antiferromagnetic phase, while a compressive strain turns the system ferromagnetic. We understood that behavior by looking at the relative displacement between layers due to the strain. We also study the evolution of the magnetic anisotropy, the magnetic exchange coupling between Cr atoms, and how the Curie temperature is affected by the strain.

MA 36.3 Wed 15:45 HSZ 101

Effect of hydrostatic pressure on the magneto-elastic coupling in 2D ferromagnet Cr₂Ge₂Te₆ — ●LAURA T. CORREDOR-BOHÓRQUEZ¹, BASTIAN RUBRECHT¹, GAËL BASTIEN¹, ANJA U. B. WOLTER¹, SEBASTIAN SELTER¹, SAICHARAN ASWARTHAM¹, and BERND BÜCHNER^{1,2} — ¹Institute for Solid State and Materials Research, Leibniz IFW Dresden, 01069 Dresden — ²Faculty of Physics, Technische Universität Dresden, Dresden

Low-dimensional magnetism is currently a rapidly developing area of research: the existing challenges in this area are mainly associated with the search and improvement of compounds whose characteristics meet the needs of innovative technologies. For exciting new applications such as ultra-compact spintronics or magnonic devices, 2D magnetic order is crucial. Following the recent re-visit of 2D ferromagnetic semiconductor Cr₂Ge₂Te₆, a full understanding of the mechanism behind its magnetism is compelling. Two main magnetic nearest-neighbor interactions are theoretically predicted: an AFM direct exchange interaction, and a FM superexchange interaction, being the ground state a result from the competition between them. In order to investigate how the magneto elastic coupling influences the physical properties of this material, we have performed hydrostatic pressure experiments. The magnetic field was applied in the c axis, i.e. the easy-magnetization axis. AFM interaction is enhanced, at the same time that there is a reduction of the FM properties, as predicted earlier from first prin-

ciple calculations. The roles of competing magnetic interactions and anisotropy with the increase of pressure are discussed.

MA 36.4 Wed 16:00 HSZ 101

Magnetic Anisotropy and Low Field Magnetic Phase Diagram of the Quasi Two-Dimensional Ferromagnet Cr₂Ge₂Te₆ — ●SEBASTIAN SELTER^{1,2}, GAËL BASTIEN¹, ANJA U. B. WOLTER¹, SAICHARAN ASWARTHAM¹, and BERND BUECHNER^{1,2} — ¹Institute for Solid State Research, Leibniz IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — ²Institute of Solid State and Materials Physics, Technische Universität Dresden, 01062 Dresden, Germany

All known quasi two-dimensional ferromagnets, such as CrX₃ (X = Br, I) and Cr₂(Ge,Si)₂Te₆, exhibit a peculiar temperature dependence of the magnetization under small external fields in the hard plane. Investigating the van der Waals layered compound Cr₂Ge₂Te₆ by magnetization and specific heat measurements under magnetic fields, we find the temperature dependence of the effective magnetic anisotropy as plausible explanation for this unusual behavior.

Based on magnetic temperature-field phase diagrams measured with magnetic fields applied along the magnetic easy axis and in the hard plane, the temperature dependence of the effective magnetic anisotropy constant was extracted and its thermal evolution was compared to the corresponding theory. A qualitative scheme is developed explaining the changes of magnetization direction due to the influence of temperature, as well as strength and direction of external magnetic fields in Cr₂Ge₂Te₆.

15 min. break.

MA 36.5 Wed 16:30 HSZ 101

Enhancement of Curie temperature in Mn₅Ge₃ films — ●YUFANG XIE^{1,2}, YE YUAN¹, HANNES SIMON FUNK³, CHI XU¹, MANFRED HELM^{1,2}, SHENGQIANG ZHOU¹, and SLAWOMIR PRUCNAL¹ — ¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden Rossendorf, Dresden 01328, Germany — ²Technische Universität Dresden, Dresden 01062, Germany — ³Institut für Halbleitertechnik, Universität Stuttgart, Stuttgart 70569, Germany

We report the effects of strain on the structural and magnetic properties of epitaxial Mn₅Ge₃ on Ge/Si (111) substrate by applying ms-range flash lamp annealing (FLA). The X-ray diffraction results demonstrate that during the FLA process the formation of nonmagnetic secondary phases of Mn_x*5Ge_y*3 is fully suppressed but the layer becomes strained. The temperature-dependent magnetization results indicate that the Curie temperature of Mn₅Ge₃ increases from 280 K up to 400 K with increasing annealing temperature. The biaxial strain generated in Mn₅Ge₃ during ms-range FLA modifies the distance between adjacent Mn atoms, which provokes the different ferromagnetic interaction between them. Consequently, the significant increase of Curie temperature is observed.

MA 36.6 Wed 16:45 HSZ 101

Defective Two-Dimensional Ferromagnetic Semiconductors: Magnetic Tailoring and Improved Stability — ●LIANG HU^{1,2,3}, YUJIA ZENG², LEI CAO³, ZICHAO LI³, CHANGAN WANG³, JUANMEI DUAN³, SLAWOMIR PRUCNAL³, and SHENGQIANG ZHOU³ — ¹College of Materials and Environmental Engineering, Hangzhou Dianzi University, Hangzhou, P. R. China — ²College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, P. R. China — ³Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany

2D ferromagnets with high Curie temperature are desirable for spintronic applications. For nonmagnetic van der Waals crystals with atomic thickness, the extrinsic tailoring such as doping or defect-engineering can render them to be ferromagnetic 2D semiconductors. Herein, we introduce three emerging 2D ferromagnetic candidates including mono-element (phosphorene and antimonene) and binary compound (MnSe₂). By applying nonmetal/metal ions doping and defect engineering, robust ferromagnetic behaviors (T_c far beyond 300 K) have been accessed by the combination of SQUID, MOKE and MFM characterization tools. Density functional theory calculations show that these defects can be stabilized in 2D systems and contribute to

net moment. Furthermore, the well-known issues of stability in thin 2D structures are also addressed, which are highly dependent on the selection of preparation and processing routes. The above merits can excite more intensive research and open a promising way to explore 2D magnets-based device applications.

MA 36.7 Wed 17:00 HSZ 101

Transitional metal doped $\text{Bi}_{2-n}\text{X}_n\text{O}_2\text{Se}$ - novel 2D magnetic semiconductor — •DOMINIK LEGUT¹, XIAOPENG LIU², RUIFENG ZHANG², ZHONGHENG FU², TINSHUAI WANG², YANCHEN FAN², and QIANFAN ZHANG² — ¹IT4Innovations, VSB-TU Ostrava, Ostrava, Czech Republic — ²School of Mat. Sci. and Eng., Beihang University, Beijing, China

For the spintronic applications like large data storages (high capacity HDD) the industry searches for ferromagnetic insulators at nanoscale size. Recently the discovery of $\text{Bi}_2\text{O}_2\text{Se}/\text{Te}$ phases that exist as 2D material and still are semiconducting attract attention. Here we investigate $\text{Bi}_{2-n}\text{X}_n\text{O}_2\text{Se}$ by transitional metal doping to introduce a magnetic spin order. We explore the electronic and magnetic properties of various ferromagnetic (e.g. Fe) or antiferromagnetic (e.g. Mn) transitional metals doped $\text{Bi}_2\text{O}_2\text{Se}$ phases within the framework of density functional theory based electronic structure calculations. We start with the magnetic order of the bulk phase in which the magnetic atoms form interlayer coupling that vary with the type and concentration of doped atoms and go towards the nanoscale dimension, i.e. 2D materials. As a result of the competitions of magnetic interactions the magnetic anisotropy energy is a crucial quantity. In combinations with Monte Carlo simulations we are able to solve the exchange interaction constants for the Heisenberg model and therefore evaluate the Curie temperature to see if these types of materials are suitable to become novel dilute magnetic semiconductors for spintronic applications at room and above temperatures.

MA 36.8 Wed 17:15 HSZ 101

DFT+HIA Description of Rare-Earth Adatoms on Graphene — •JOHANNA P. CARBONE^{1,2}, HENNING JANSSEN¹, GUSTAV BIHLMAYER¹, ALEXANDER B. SHICK⁴, MARIA PERESSI³, and STEFAN BLÜGEL¹ — ¹PGI-1/IAS-1 Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — ²Department of Chemical and Pharmaceutical Sciences, University of Trieste, I-34127 Trieste, Italy — ³Department of Physics, University of Trieste, I-34127 Trieste, Italy — ⁴Institute of Physics ASCR, CZ-18221 Prague, Czech Republic.

Composite 2D-materials containing rare-earth atoms are interesting candidates for quantum technology thanks to their large magnetic moments, rich magnetic interactions and strong spin-orbit coupling effects. The main problem in describing these systems in density functional theory (DFT) using the conventional approximations lies in the strongly localized and correlated 4f-electrons. A promising path is the combination of DFT with the Hubbard-I approximation [1] to the Anderson impurity (DFT+HIA) [2]. The DFT-HIA model has been recently implemented into the FLAPW code FLEUR

(www.juDFT.de). Preliminary tests on systems containing lanthanide adatoms on graphene have shown promising results. The goal is now to study complex magnetism and effects such as magnetic anisotropy in novel 2D-materials containing layers of lanthanides intercalated between sheets of van der Waals heterostructures.

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[1] Shick et al., Phys. Rev. B 80, 085106 (2009)

[2] Kolorenč et. al., Phys. Rev. B 92, 085125 (2015)

MA 36.9 Wed 17:30 HSZ 101

Enhanced indirect exchange interactions in the presence of circular potentials in graphene — •OZGUR CAKIR and AHMET UTKU CANBOLAT — Izmir Institute of Technology, Physics Department, 35430, Urla, Izmir, TURKEY

We study indirect exchange interaction between two magnetic impurities in pristine graphene in the presence of a circular potential. In bulk graphene structures indirect exchange interaction, also known as RKKY (Ruderman-Kittel-Kasuya-Yosida) interaction, shows a power-law decay with distance for both doped and undoped cases. Here we show that under a circular electric potential quasibound states lead to enhanced RKKY interactions between magnetic moments located in the vicinity of the potential well. It is shown that the strength of the potential well and Fermi energy can be tuned to create enhanced long ranged RKKY interactions. We show that when the Fermi level lies at the quasibound state energy, the scattering processes between the states of the same chirality dominate over the other scattering channels and this leads to a predominantly ferromagnetic, enhanced interaction between the impurities at long distances. The predicted effect can enable electrical control of RKKY interactions in graphene or other two-dimensional materials.

MA 36.10 Wed 17:45 HSZ 101

Ferromagnetism in graphene — •MUKUL KABIR — Department of Physics, Indian Institute of Science Education and Research, Pune 411008, India

Metal-free magnetism in graphene has remained a subject of intense research, and many research groups have invested in understanding the roles of doping, structural defects and edge structure in finite-sized nano-flakes. However, a robust long-range magnetic order has remained elusive. In this context, recently nitrogen-doped graphene is experimentally proposed to be a promising candidate, however, the Curie temperature remains controversial. The corresponding exchange mechanism endures unclear and is essential to tune further and manipulate magnetism. In this talk, within the first-principles calculations, we will systematically discuss the local moment formation and the concurrent interaction between various defect complexes. The importance of adatom diffusion on the differential defect abundance will be elaborated. We will establish that the direct exchange mechanism between the delocalized magnetic moment originating from the π -electron at the prevalent triazine complex to be responsible for the observed ferromagnetism.