Magnetic Interfaces and Nanostructures
Room 101C - Session MI+2D+AC-MoA

Magnetism and Spin Orbit Effects at Interfaces and Surfaces: Recent Experimental and Theoretical Advances

Moderator: Valeria Lauter, Oak Ridge National Laboratory

1:40pm **MI+2D+AC-MoA1 Bi-$_1$Te$_1$: A New Dual Topological Insulator**, ***Lukasz Plucinski***, *M. Eschbach, M. Lanius, C. Niu, E. Mlynczak, P. Gospodaric,* FZ Jülich GmbH, Germany*; J. Kellner,* RWTH Aachen University, Germany*; P. Schüffelgen, M. Gehlmann, S. Döring, E. Neumann, M. Luysberg, B. Holländer, G. Mussler,* FZ Jülich GmbH, Germany*; M. Morgenstern,* RWTH Aachen University, Germany*; D. Grützmacher, G. Bihlmayer, S. Blügel, Schneider,* FZ Jülich GmbH, Germany

We present, a combined theoretical and experimental study on the prediction and verification of the dual topological insulating character of the stoichiometric natural superlattice phase $Bi_1Te_1 = [Bi_2]_1[Bi_2Te_3]_2$ [1]. We identify Bi_1Te_1 by density functional theory to exhibit a non-trivial time-reversal symmetry-driven character of Z_2 = (0; 001) and additionally a mirror-symmetry induced mirror Chern number of ν_{M-} = -2, which indicates that Bi_1Te_1 is both a weak topological insulator (WTI) and a topological crystalline insulator (TCI). The coexistence of the two phenomena preordain distinct crystal planes to host topological surface states that are protected by the respective symmetries. From the analysis of time-reversal invariant momenta (TRIM-points) the surface perpendicular to the stacking direction, for instance, is found as the time-reversal symmetry *dark* surface, while hosting mirror-symmetry protected non-TRIM surface states along the surface-Gamma-M direction. We confirm the stacking sequence of our MBE-grown Bi_1Te_1 thin films by X-ray diffraction and transmission electron microscopy (STEM), and find clear indications of the TCI and WTI character in the surface electronic spin structure by spin- and angle-resolved photoemission spectroscopy.

[1] M. Eschbach et al., arXiv:1604.08886 (2016).

2:00pm **MI+2D+AC-MoA2 Spin-Polarized Scanning Tunneling Microscopy of a Two-Dimensional Ferromagnetic Semiconductor at Room-Temperature**, ***Yingqiao Ma***, *A.R. Smith,* Ohio University*; A. Barral, V. Ferrari,* Centro At´omico Constituyentes, GIyA, CNEA, Argentina

Ferromagnetic semiconductors are very promising materials for the spintronic applications, as they are good spin-polarized carrier sources and easy to be integrated into semiconductor devices. The search for ferromagnetic semiconductors with Curie temperature above the room-temperature has been a long-standing goal, since the Curie temperature *Tc* of most ferromagnetic semiconductors are at the cryogenic level with little possibility of improvement, which hinders their future practical spintronic applications.

Here, we observed the ferromagnetic domain structure at room-temperature on a GaN-based two-dimensional MnGaN semiconducting surface alloy, using spin-polarized scanning tunneling microscopy/spectroscopy which is sensitive to the surface magnetic nanostructures and can completely rule out the extrinsic origin of the ferromagnetism such as magnetic elements segregation by its ultimate spatial resolution. In contrast to the randomly doped dilute magnetic semiconductors, the two-dimensional surface structure has a unique and well-ordered hexagonal-like Mn √3 x √3 - R30° symmetry. The total density of states of the Mn √3 x √3 - R30° structure calculated by the density functional theory agree well with our normalized differential tunneling *dI/dV* spectroscopy, which clearly reveal the spin-polarized and spin-split Mn surface density of states peaks and prove the semiconducting nature of the surface as the normalized *dI/dV* goes to zero at the Fermi level. By applying a small magnetic field to the sample, the magnetic hysteresis is mapped out, which further proves its ferromagnetic nature. In conclusion, we demonstrated the room-temperature ferromagnetic nature of the two-dimensional Mn √3 x √3 - R30° structure, which makes it a promising material for future realistic magnetic storage, field-controlled, and quantum computing nano spintronic devices.

2:20pm **MI+2D+AC-MoA3 Spin-Orbit Induced Surface States of Rashba Systems and Topological Insulators**, ***Peter Krüger***, *T. Förster, M. Rohlfing, P. Eickholt, A.B. Schmidt, M. Donath,* Westfälische Wilhelms-Universität Münster, Germany **INVITED**

The generation of spin-polarized electrons on the basis of spin-orbit coupling at the surfaces of nonmagnetic solids has attracted considerable interest in recent years. Adlayers of heavy atoms, in particular, give rise to an interesting physics of spin-split surface states going far beyond the simple Rashba model. However, only very few studies have been reported that address unoccupied states of these systems, despite their relevance for potential applications. In the first part of this contribution, we present results from ab-initio calculations as well as spin- and angle-resolved inverse photoemission (IPE) for systems showing empty bands with a giant spin splitting and a unique structure of the spin polarization. For Tl/Si(111) and Tl/Ge(111), we identify spin-split states whose polarization vector rotates from the Rashba direction to an out-of-plane polarization when going from Gamma to K. Surprisingly, the spin splitting of the bands on Tl/Ge(111) is much smaller than on Tl/Si(111) despite the stronger surface localization and the heavier substrate. Our detailed analysis of the electronic structure shows that a remarkable interplay between spin-orbit coupling and hybridization is responsible for this unexpected result. Furthermore, we notice a distinct spin asymmetry in the intensity of the measured spectra at M, a time-invariant k-point. Our simulations of the IPE process unravel this puzzling behavior.

In the case of topological insulators, spin-orbit coupling gives rise to topologically protected surface states. We identify problems of the widely used density-functional theory (DFT) with a proper description of these states and demonstrate that they can be overcome by employing the GW self-energy operator within ab initio many-body perturbation theory. In particular we have investigated thin films of Bi2Se3, Bi2Te3, and Sb2Te3 with thicknesses from one to six quintuple layers. The quasiparticle band structures show highly improved agreement with experiments compared to DFT. In addition to a correction of the band gaps, the energetic positions and dispersions of the surface states change significantly around the Dirac point. As the wave functions are updated in our approach, the two-dimensional topological phases (quantum spin Hall or trivial) in GW can be different from the DFT result. We find the nontrivial quantum spin Hall phase, together with a sizable band gap 0.13 eV for a Bi2Te3 slab of 2 QL thickness.

[1] P. Eickholt et al., Phys. Rev. B 93, 085412 (2016)

[2] T. Förster et al., Phy. Rev. B 92, 291404 (R) (2015)

3:00pm **MI+2D+AC-MoA5 Spin-Resolved Momentum Microscopy of Strongly Correlated Electron Systems and Topological Insulators**, ***Christian Tusche***, Forschungszentrum Jülich, Germany **INVITED**

One of the fundamental concepts in solid state physics is the description of the degrees of freedom of the electrons in the solid by the relation of the energy E vs. the crystal momentum k in a band structure of quasi particles. Of particular importance is the spin of the electron that leads to phenomena like ferromagnetism, spin-polarized surface- and interface-states, and recently, the discovery of new material classes like topological insulators. The latter attracted wide interest by the unusual relations of electron-spin and -momentum. In addition, strong spin-orbit coupling also leads to a rich band-structure of highly polarized states beyond the well known "Dirac cone" surface state. A direct conclusion on the ground state polarization in these systems is rather complicated by the peculiar interplay between spin- and light-polarization, as directly observed in spin-resolved photoemission maps over the full surface Brillouin zone .

On the experimental side, the novel concept of momentum microscopy evolved to provide an intuitive and comprehensive insight to these band structures. A momentum microscope captures the complete 2π solid angle of emitted photoelectrons into a high resolution image of electronic states in reciprocal space [1]. With the introduction of imaging spin analyzers, the efficiency of spin-resolved measurements experienced a tremendous boost [2]. Together with modern synchrotron radiation sources, delivering photon energies from UV to soft X-rays as well as a flexible timing structure, the electron spin now becomes routinely accessible in photoemission experiments. In particular, new developments like time-of-flight momentum microscopy now provide comprehensive three-dimensional data sets of the complete valence band region within a single measurement [3]. Here, we discuss examples and prospects of spin resolved momentum microscopy, ranging from tomographic imaging of the spin-resolved Fermi surface of ferromagnets to the rapid band-structure mapping of novel materials.

[1] C. Tusche, A. Krasyuk, J. Kirschner: Ultramicroscopy 159, p. 520 (2015),

[2] C. Tusche, M. Ellguth, A. A. Ünal, C.-T. Chiang, A. Winkelmann, A. Krasyuk, M. Hahn, G. Schönhense, J. Kirschner: Appl. Phys. Lett. 99, 032505 (2011)

[3] C. Tusche, P. Goslawski, D. Kutnyakhov, M. Ellguth, K. Medjanik, H. J. Elmers, S. Chernov, R. Wallauer, D. Engel, A. Jankowiak, G. Schönhense: Appl. Phys. Lett., in press (2016)

4:00pm **MI+2D+AC-MoA8 Spin-orbit-Induced Effects in the Electronic Structure of W(110) and Ta(110): Similarities and Differences**, ***Markus Donath**, K. Miyamoto, H. Wortelen, B. Engelkamp,* Muenster University, Germany*; H. Mirhosseini,* Max Planck Institute for Microstructure Physics, Germany*; T. Okuda,* Hiroshima Synchrotron Radiation Center, Japan*; A. Kimura,* Hiroshima University, Japan*; A.B. Schmidt,* Muenster University, Germany*; J. Henk,* Martin Luther University Halle-Wittenberg, Germany

Tungsten and tantalum are direct neighbors in the periodic table and exhibit, at first glance, a very similar electronic structure. Only the bands of tantalum are less occupied due to the lack of one electron. For W(110), an exceptional surface state was discovered [1]: Resembling a topological surface state (TSS), it exhibits a linear dispersion with a helical spin texture in reciprocal space, often called Dirac-cone-like behavior. Interestingly and again reminiscent of the TSS behavior, photoemission calculations predict a spin reversal upon changing the light polarization used for excitation from *p* to *s* [2]. We verified this orbital-symmetry-selective spin texture by spin-resolved photoemission [3]. This result unveils, in which way spin-orbit interaction entangles spin and orbital degrees of freedom. “Spin control” is not restricted to topological insulators but a much more general phenomenon.

A surface state, similar to the Dirac-cone-like state on W(110), may be expected for Ta(110), yet above the Fermi level. Surprisingly, our spin-resolved inverse-photoemission results do not show this state. Instead, spin-polarized unoccupied surface bands [4] and an occupied d_{z^2}surface state with Rashba-like spin texture [5] were identified, which have no equivalents on W(110). These findings are explained by subtle differences in the energetic positions of the surface states relative to the bulk states for W(110) and Ta(110), which critically depend on the values for the lattice constant and the surface relaxation.

[1] K. Miyamoto *et al.*, Phys. Rev. Lett. **108**, 066808 (2012); Phys. Rev. B **86**, 161411(R) (2012); J. Electron Spectrosc. Relat. Phenom. **201**, 53 (2015).

[2] H. Mirhosseini *et al.*, New J. Phys. **15**, 033019 (2013).

[3] K. Miyamoto *et al.*, Phys. Rev. B **93**, 161403(R) (2016).

[4] B. Engelkamp *et al.*, Phys. Rev B **92**, 085401 (2015).

[5] H. Wortelen *et al.*, Phys. Rev. B **92**, 161408(R) (2015).

4:20pm **MI+2D+AC-MoA9 Formation of a 2D Interface by Low Energy Proton Implantation in ZnO Microwires**, ***Israel Lorite**, Y. Kumar,* Universität Leipzig, Germany*; B. Straube, S. Perez,* Universidad Nacional de Tucumán, Argentina*; C. Rodriguez,* Universidad Nacional de La Plata, Argentina*; P. Esquinazi,* Universität Leipzig, Germany

Recently we showed the possibility of obtaining room temperature magnetic order by implanting protons (H+) at low energies (300 V) into Li-doped ZnO microwires [1]. The low energy implantation is enough to produce Zn vacancies (V_{Zn}) within 10 nm from the surface, without creating too much disorder in the ZnO lattice. The formation of a stable density of defects in the 10 nm depth region is possible since Li doping reduces the energy of stabilization of V_{Zn}. Thus, the concentration of V_{Zn} will be approximately the one of the Li doping. Along with the observation of magnetic order at room temperature, the ZnO microwires present an anomalous temperature dependence of the negative magnetoresistance. Such a behavior can be related to the formation of an interface at the boundary between the magnetic and non-magnetic structure produced by the implantation. In this contribution we show the observation of a photo-galvanic effect related to the Rashba effect. This effect is due to the formation of a 2D electron gas at the interface of the magnetic/non-magnetic structure. In addition, an increase of this effect is observed by the application of a small external magnetic field, related to the existence of a 10 nm magnetic region produced during the proton irradiation.

[1] I.Lorite, et al; Advances in methods to obtain and characterize room temperature magnetic, Appl. Phys. Lett. 106, 082406 (2015)

4:40pm **MI+2D+AC-MoA10 Density Functional Studies of Magnetic and Spintronic Materials**, ***Ruqian Wu**,* University of California Irvine **INVITED**

Magnetism, one of the oldest branches of physics, is having its renaissance in recent years due to the interest in developing various nanomagnets, molecular magnets and magnetic nanojunctions for the development of innovative devices. Magnetization of surfaces and nanostructures is sensitive to the change of environment and hence the availability of ultrahigh vacuum is crucial for the exploration of various magnetic systems. Equally important is the rapid advance of density functional theory (DFT) approaches, which now can reliably predict large amount physical properties of real materials in either their ground states or excited states. In this talk, I will discuss several our recent theoretical progresses in spin-related physics, including 1) the search for giant magnetic anisotropy energy in nanostructures; 2) the design to imprint large spin orbit coupling into graphene and other two-dimensional materials for the realization of quantum spin Hall effect and quantum anomalous Hall effect; 3) the photo-spin-voltaic effect; and 4) the generation of spin-polarized two-dimensional electron gas at oxide interfaces. Most of our DFT studies are performed in close collaboration with experimental groups so some experimental results will also be discussed.

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