O 57: Focused Session: Spin-Orbit Interaction at Surfafces: From the Rashba Effect to Topological States of Matter II

Time: Thursday 15:00–19:00 Location: HSZ 02

Topical Talk O 57.1 Thu 15:00 HSZ 02
Rashba-type spin-orbit effects by spin-resolved photoemission — •Oliver Rader — Helmholtz-Zentrum Berlin

In order to create spin currents in a solid, the Rashba effect can be instrumental. It requires neither a ferromagnetic material nor external magnetic fields. In this talk, we show that a quantum cavity for spin can be constructed from metals. Spin- and angle-resolved photoemission is used to study the dependence of the spin-orbit splitting of quantum-well states on parameters such as momentum and atomic number. In this context, we will also discuss the perspectives of graphene for spintronics.

Topical Talk O 57.2 Thu 15:30 HSZ 02
Quantum spin Hall phases and topological surface states — •Shuichi Murakami — Department of Physics, Tokyo Institute of Technology, Tokyo, Japan — PRESTO, JST

Triggered by the research of the spin Hall effect [1], quantum spin Hall (QSH) effect [2,3] is studied intensively in recent years. The QSH system is an insulator in the bulk, while the boundary (i.e. edge in 2D and surface in 3D) supports gapless states carrying spin currents due to spin-orbit coupling. These edge or surface states remain gapless, and are robust against nonmagnetic impurities and surface roughness. This robustness stems from bulk topological order characterized by the Z_2 topological number. Namely, the bulk topological properties become manifest as an existence of the gapless boundary states.

The QSH effect occurs under a zero magnetic field unlike the quantum Hall effect. In some materials this effect occurs in nature without applying fields, as demonstrated theoretically and experimentally. In my talk I explain our theoretical proposal that the (111)1-bilayer bismuth ultrathin film shows the QSH effect [4]. I also discuss strategies to search for candidate materials showing the QSH effect.

[1] S. Murakami, N. Nagaosa, and S.-C. Zhang, Science 301, 1348 (2003). [2] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802; ibid. 95, 226801 (2005). [3] B. A. Bernevig and S.-C. Zhang, Phys. Rev. Lett.96.106802 (2006). [4] S. Murakami, Phys. Rev. Lett. 97, 236805 (2006).

Topical Talk O 57.3 Thu 16:00 HSZ 02
Observation of a new topological phase of quantum matter : Quantum Hall-like effect without magnetic field. — •Zahid Hasan — Princeton University, Princeton, New Jersey, USA

Most quantum states of condensed-matter are categorized by the spontaneously broken symmetries. The remarkable discovery of charge quantum Hall effects (1980s) revealed that there exists an organizational principle of matter based not on the spontaneously broken symmetry but only on the topological distinctions in the presence of time-reversal symmetry breaking. In the past few years, theoretical developments suggest that new classes of topological states of matter might exist that are purely topological in nature in the sense that they do not break time-reversal symmetry hence can be realized without any applied magnetic field : "Quantum Hall-like effects without magnetic field". In this presentation, I report a series of experimental results documenting and demonstrating the existence of such a topologically ordered time-reversal-invariant state of matter and discuss the exotic electromagnetic and spin properties this novel phase of quantum matter might exhibit and outline their potential use.

O 57.4 Thu 16:30 HSZ 02
Rashba type spin-orbit splitting of quantum well states in ultrathin Pb films — •Hugo Dil[1,2], Fabian Meier[1,2], Jorge Lobo-Checa[3], Luc Patthey[2], Gustav Bihlmayer[4], and Jürg Osterwalder[1] — [1]Universität Zürich, CH — [2]Swiss Light Source, CH — [3]Universität Basel, CH — [4]Forschungszentrum Jülich, D

When the thickness of a metal layer approaches the electron coherence length, quantum well states (QWS) may form in the layer. It has been shown previously that QWS may show a spin splitting due to hybridization with interface[1] or surface states[2], which either decays with layer thickness or is sensitive to contamination. Here we will report the first observation of an intrinsic Rashba type spin-orbit splitting in metallic QWS by spin and angle-resolved photoemission[3]. The resulting band splitting is too small to be detected by spin integrated ARPES and highlights the possibilities of state-of-the-art spin resolved ARPES. It will be shown that the spin-orbit interaction takes place throughout the whole layer, but that the necessary asymmetry is induced by the two interfaces of the film. This opens up the possibility to manipulate the effect by interface engineering.

[1] C. Koitzsch et al. PRL 95, 126401 (2005)
[2] K. He et al. PRL 101, 107604 (2008); E. Frantzeskakis et al. PRL 101, 196805 (2008)
[3] H. Dil et al. PRL in press

O 57.5 Thu 16:45 HSZ 02
Relativistic effects in the surface emission of layered intermetallic systems — •Jurgen Braun, Jan Minar, Sven Bornemann und Hubert Ebert — Dep. Chemie und Biochemie, LMU München, Germany

In the framework of the fully relativistic version of the one-step model, the photoemission intensities resulting from layered intermetallic thin films will be presented. The electronic structure as well as the photoemission calculations have been performed for true semi-infinite systems using the upgraded version of the Munich SPR-KKR program package [1]. To guarantee for a quantitative description of the surface-sensitive spectral distribution special attention is payed on the image-potential behavior of the surface barrier, which is included as an additional layer in the photoemission formalism [2]. Here, we show the intensity distributions that result by excitation with ultraviolet radiation from Ag/Au(111), Ag/Au(110) and Au/Ni(111) surfaces. We discuss the variation in binding energy and spin-orbit splitting of the corresponding surface states as a function of the overlayer thickness and compare our results with available experimental data.

1. H. Ebert et al., The munich SPR-KKR package, version 3.6, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2008).
2. A. B. Schmidt et al., J. Phys. D: Appl. Phys. **41** 164003 (2008).

O 57.6 Thu 17:00 HSZ 02
Ab initio *g*-tensor calculation for paramagnetic surface states — •Martin Rohrmüller[1], Uwe Gerstmann[1,2], and Wolf Gero Schmidt[1] — [1]Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Institut de Minéralogie et de Physique des Milieux Condensés, Université Pierre et Marie Curie, Campus Boucicaut, 140 rue de Lourmel, 75015 Paris, France

The effects of spin-orbit interaction provide an interesting possibility to investigate the electronic and microscopic structure at surfaces. The spin-orbit coupling determines e.g. the elements of the electronic g-tensors which can be observed in electron paramagnetic resonance (EPR) measurements. Based on double-perturbation theory we are able to calculate the g-tensor from first principles, using a recently developed gauge-including projector augmented plane wave (GI-PAW) approach [1] in the framework of density functional theory.
The presented approach is able to distinguish between different surface states. In combination with the corresponding experimental EPR data an unambiguous identification of the microscopic structure of adsorped species becomes possible. This is demonstrated here for surface defects at hydrogen-passivated Si(001) and Si(111) surfaces.

[1] Ch.J. Pickard and F. Mauri, Phys. Rev. Lett. **88**, 086403 (2002).
[2] U. Gerstmann, A. P. Seitsonen and F. Mauri, phys. stat. sol. (b) **245**, 924 (2008).

O 57.7 Thu 17:15 HSZ 02
Bi(114): A quasi one-dimensional metal with strong spin-orbit splitting — •Philip Hofmann[1], Justin Wells[1,2], Hugo Dil[3,4], Fabian Meier[3,4], Jorge Lobo-Checa[3,4], Vladimir Petrov[5], Jürg Osterwalder[3], Miguel Moreno Ugeda[6], Isabel Fernandez-Torrente[6], Jose Ignacio Pascual[6], Emile Rienks[1], and Maria Fuglsang Jensen[1] — [1]University of Aarhus, DK — [2]University of Science and Technology, Trondheim, N — [3]Universität Zürich-Irchel, CH — [4]Paul Scherrer Institut, CH — [5]St. Petersburg Technical University, RU — [6]Freie Universität Berlin, D

The (114) vicinal surface of the semimetal Bi is found to support a quasi one-dimensional, metallic surface state. As required by symmetry, the state is degenerate along the $\bar{\Gamma}-\bar{Y}$ line of the surface Brillouin zone with a highest binding energy of ≈100 meV. In the $\bar{\Gamma}-\bar{X}$ direction the degeneracy is lifted by the strong spin-orbit interaction, as directly shown by spin-resolved photoemission. This results in a Fermi surface consisting of two closely separated, paralell lines of opposite spin direction. We discuss these findings in the light of the recently discovered topological stability of surface states on BiSb topological insulators.

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O 57.8 Thu 17:45 HSZ 02

Spin restrictions in the electron interference process on Bi(110) — •Anna Strozecka[1], Asier Eiguren[2], and Jose Ignacio Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 Donostia/San Sebastian, Spain

The surfaces of bismuth can be viewed as a quasi-two-dimensional metal with unique spin properties [1]. The strong spin-orbit interaction and the lack of the symmetry on the surface results in the splitting of the surface state bands with respect to the spin direction. The lack of the spin degeneracy strongly affects the quasiparticle interference [2]. We have studied in detail the interference patterns on Bi(110) surface by means of scanning tunneling microscopy. The observed patterns do not reflect directly the shape of the Fermi contour, as it is usually found for metals, but result from the spin-conserving scattering process. The investigation of the energy dependence of the interference reveals that at the energies away from the Fermi level highly anisotropic patterns arise. The origin of theses new scattering events can be established by analyzing the dispersion of the spin split bands. The interpretation of the data is supported by spin-resolved DFT simulations.

[1] Ph. Hofmann, Prog. Surf. Sci. 81, 191 (2006)
[2] J. I. Pascual et. al., Phys. Rev. Lett. 93, 196802 (2004)

O 57.9 Thu 18:00 HSZ 02

Spin-orbit coupling effect on surface state ripples — •Samir Lounis, Andreas Bringer, and Stefan Blügel — Institut für Festkörperforschung and Institut for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

Surfaces are an inversion asymmetric environment. In combination with the spin-orbit interaction, surface electrons experience a Rashba effect, which leads to spin-split surface states. Having an adatom on such a surface, surface states scatter at it. Interferences are created from which, surprisingly, the fingerprints of spin-orbit coupling cannot be seen with a scanning tunneling microscope (STM) [3]. Instead of a single adatom, Walls and Heller [4] proposed to use a corral of atoms to create extra spin-orbit coupling related modulations in the charge density. Resting on multiple scattering theory, we propose a different suggestion to visualize such effects using STM considering either a single adatom or a corral of adatoms.

This work is supported by the ESF EUROCORES Programme SONS under contract N. ERAS-CT-2003-980409 and the DFG Priority Programme SPP1153.

[1] S. Lashell, B.A. McDougall, E. Jensen, Phys. Rev. Lett. **77**, 3419 (1996).
[2] Yu. M. Koroteev, G. Bihlmayer, J.E. Gayone, E.V. Chulkov, S. Blügel, P.M. Echenique, Ph. Hofmann, Phys. Rev. Lett. **93**, 046403 (2004).
[3] L. Petersen and P. Hedegård, Surf. Sci. **49**, 459 (2000).
[4] J.D. Walls and E.J. Heller, Nano Letters **7**, 3377 (2007).

O 57.10 Thu 18:15 HSZ 02

An ab-initio description of the magnetic shape anisotropy — •Sven Bornemann, Jan Minar, Jürgen Braun, and Hubert Ebert — Department Chemie und Biochemie, LMU München, Germany

For magnetic transition metal systems with reduced dimensionality and low symmetry the shape anisotropy becomes a significant contribution to the magnetic anisotropy. In fact, it can reach the same order of magnitude as the spin-orbit induced anisotropy. So far, the shape anisotropy has been always treated as a classical interaction between magnetic dipoles while the spin-orbit anisotropy has been determined by relativistic band structure calculations. It is uncertain, however, whether such an inconsistent treatment of the two anisotropy contributions is still valid for low dimensional nano structures such as magnetic thin films, wires or clusters where the magnetic easy axis can depend strongly on the interplay between these two contributions.

As an alternative to the classical approach an ab-initio description of the shape anisotropy has been developed. This is achieved by including the Breit interaction, being the natural cause of the shape anisotropy, in the Dirac-equation set up within the framework of spin density functional theory. We have implemented this approach using the fully relativistic KKR band structure scheme. We will present the details of our implementation and show first results for the shape anisotropy of thin Fe films on Au(001) in comparison with the classical treatment.

O 57.11 Thu 18:30 HSZ 02

Spin-orbit induced exchange interactions in magnetic surfaces described by first-order perturbation theory — •Marcus Heide, Gustav Bihlmayer, and Stefan Blügel — Institut für Festkörperforschung (IFF) and Institute of Advanced Simulation (IAS), Forschungszentrum Jülich, Germany

When applying the spin-orbit coupling operator $H_{\rm so}$ as a perturbation to a Schrödinger-type equation, the first-order term $\sum_\nu \langle\psi_\nu|H_{\rm so}|\psi_\nu\rangle$ vanishes for all collinear magnetic structures. Thus, the magnetocrystalline anisotropy is at least a second-order effect in the spin-orbit coupling and cannot be calculated from the expectation values of $H_{\rm so}$. However, in systems with low magnetic and spatial symmetry these expectation values do not necessarily vanish: Non-collinear magnetic structures in surface geometries allow for magnetic interactions of Dzyaloshinskii-Moriya type, that are first order in $H_{\rm so}$. These interactions can have a significant impact on the magnetic structure of low-dimensional magnets [M. Bode *et al.*, Nature **447**, 190 (2007)].

In this talk, we investigate the role of the spin-orbit coupling in ultrathin Fe and Mn films on transition metal surfaces in the framework of density functional theory. Employing the `FLEUR` code (www.flapw.de), we compare the expectation values of $H_{\rm so}$ with the higher-order corrections and show that first-order perturbation theory is capable of estimating the antisymmetric exchange interactions in these systems. This allows to use simple models to relate these interactions to the electronic structure. This work is supported by DFG (BI 823/1-1) and ESF EUROCORES Programme SONS (ERAS-CT-2003-980409).

O 57.12 Thu 18:45 HSZ 02

Non-collinear magnetism in two-dimentional FePt systems — •Svitlana Polesya, Sven Bornemann, Sergiy Mankovsky, Jan Minar, and Hubert Ebert — Ludwig-Maximilians-Universität München, Department Chemie und Biochemie/Physikalische Chemie, München, Deutschland

The temperature dependent magnetism of a FePt monolayer and of a FePt two-dimentional (2D) alloy cluster on a Pt(111) substrate were investigated by means of Monte Carlo simulations. The calculations were based on the extended Heisenberg model accounting for isotropic exchange as well as the anisotropic Dzyaloshinski-Moriya (DM) exchange interaction. The DM coupling was found to be responsible for a non-collinear spin configuration in both alloy systems at low temperature. The Fe-Pt exchange turned out to play an important role stabilising the ferromagnetic order and appreciably influencing the critical temperature. For this reason a corresponding term in the model Hamiltonian was included describing the induced Pt magnetic moment as a function of the average magnetic moments of the surrounding Fe atoms. The role of the magnetic anisotropy on magnetic order in the 2D alloy systems was also investigated in detail.