

Wednesday Afternoon, November 8, 2023

Magnetic Interfaces and Nanostructures Division Room B110-112 - Session MI+2D+TF-WeA

Special Symposium on Coupling Phenomena in Magnetism

Moderator: Hendrik Ohldag, Lawrence Berkeley National Laboratory

2:20pm **MI+2D+TF-WeA-1 Coupling Spin-Orbit and Exchange Interaction in a Low-Dimensional Magnet**, *Pascal Jona Grenz¹, M. Donath, P. Krüger*, University of Münster, Germany

Coupling exchange interaction (SOI) and spin-orbit interaction (XCI) provides the foundation for many prospective spin-based information technology applications. For example, it was suggested that the strength of SOI at a ferromagnet/heavy-metal (FM/HM) interface is decisive for the efficiency of writing magnetic bits in spin-orbit-torque MRAM devices [1].

Exploring the electronic structure is the key to access the factors underlying the coupling of SOI and XCI. We use spin- and angle- resolved inverse photoemission to study the interplay of SOI and XCI in the unoccupied electronic structure at the interface of a low-dimensional FM on a HM substrate. The prototypical FM/HM hybrid system Ni/W(110) exhibits exchange-split Ni-related states that become strongly influenced by SOI. A balanced ratio of SOI and XCI results in a magnetization- and k-dependent quenching or enhancement of the spin splitting. This remarkably large interplay of SOI reflected in the adlayer states contrasts previous studies of the occupied electronic structure of the same system, where the observations were attributed solely to either SOI or XCI [2].

Using density-functional-theory (DFT) calculations, we investigate the underlying drivers responsible for the experimentally observed coupling of SOI and XCI. We find that hybridization between adsorbate and substrate states, along with the strongly localized wave functions at the heavy W nuclei, cause the strong influence of SOI within the Ni-related exchange-split states.

[1] I.M. Miron *et al.*, Nature, **476** 189 (2011)

[2] A. Nuber, PhD Thesis (University of Würzburg, Germany, 2011)

2:40pm **MI+2D+TF-WeA-2 AVS Graduate Research Awardee Talk: Temperature Dependent Magnetic and Electronic Properties of NiCo₂O₄ Thin Film Surfaces**, *Arjun Subed^{2,3}*, University of Nebraska-Lincoln; *D. Yang, C. Mellinger, X. Xu*, University of Nebraska-Lincoln; *P. Dowben*, University of Nebraska-Lincoln

Although NiCo₂O₄ thin film is shown to possess perpendicular magnetic anisotropy [1], we have observed in-plane spin polarization of NiCo₂O₄ thin film in spin polarized inverse photoemission spectroscopy (SPIPES). The unoccupied states of NiCo₂O₄, above Fermi level, were observed to have unequal density of states for spin majority and spin minority carriers in SPIPES, and the spectra obtained from the SPIPES have spectral features that can be compared to the XMCD spectra. The in-plane spin polarization of NiCo₂O₄ is found to decrease with increasing temperature, as expected. In addition to the temperature dependent change in spin polarization, we observed that there is change in the surface electronic properties of NiCo₂O₄ from conducting to insulating when the temperature is increased. X-ray photoemission spectroscopy (XPS) studies show that there exist no appreciable binding energy changes of Ni 2p_{3/2} and Co 2p_{3/2} core levels with change in temperature (T) when the NiCo₂O₄ film exists in conducting phase. However, when the NiCo₂O₄ films became insulating, the core level binding energies changed reversibly with change in temperature during annealing and cooling cycles. The core level binding energy (BE) change with temperature (T) is found to closely follow a modified Arrhenius type model. The proposed model is also followed by Co 2p_{3/2} and Fe 2p_{3/2} core levels in temperature dependent XPS of insulating CoFe₂O₄ thin films. Our studies indicate that thermal effects and oxygen defects should play the roles in changing both magnetic and electronic properties of NiCo₂O₄ thin films with temperature.

[1] C. Mellinger *et al.*, Phys. Rev. B **101**, 014413 (2020).

3:00pm **MI+2D+TF-WeA-3 Antiferromagnetic Real-Space Configuration Probed by Dichroism in Scattered X-Ray Beams with Orbital Angular Momentum**, *Sophie Morley, M. McCarter, A. U. Saleheen, A. Singh*, Lawrence Berkeley Lab; *R. Tumbleson*, University of California Santa Cruz; *J. Woods*, Argonne National Laboratory; *A. Tremsin*, UC Berkeley; *A. Scholl*, Lawrence Berkeley Lab; *L. de Long, J. Hastings*, University of Kentucky; *S. Roy*, Lawrence Berkeley Lab

INVITED

X-ray beams with orbital angular momentum (OAM) are a promising tool for x-ray characterization

techniques. Beams with OAM have an azimuthally varying phase, and new material properties can

potentially be probed by utilizing this unique phase structure. Here, we show how OAM beams are

created through resonant diffraction from an artificial antiferromagnet with a topological defect. The

scattered OAM beams have circular dichroism whose sign is coupled to the phase of the beam [1]. Using

magnetic scattering calculations, we show that this dichroism is related to the real-space configuration

of the antiferromagnetic ground state. Thermal cycling of the artificial antiferromagnet can change the

ground state, as indicated by the changing dichroism. These results exemplify the potential of OAM

beams to probe matter in a way that is inaccessible using currently available x-ray techniques.

[1] M. R. McCarter *et al.*, Phys. Rev. B **107**, L060407 (2023)

5:00pm **MI+2D+TF-WeA-9 Spin-dependent Hybridization of Image-potential States with TI States in TI/Ag(111)**, *Sven Schemmelm⁴*, Universität Münster, Germany; *P. Härtl*, Universität Würzburg, Germany; *P. Krüger*, Universität Münster, Germany; *M. Bode*, Universität Würzburg, Germany; *M. Donath*, Universität Münster, Germany

The BiAg₂ and PbAg₂ surface alloys exhibit giant Rashba splittings [1-4]. The related TlAg₂ surface alloy is expected to show states with smaller but still large Rashba splittings due to the lower atomic number of Tl. However, this alloy forms only small patches with long-range structural order [5]. For higher coverages of Tl on Ag(111), a smooth and stable wetting layer forms with a moiré superstructure due to the lattice mismatch between Tl and Ag. We present a study of the unoccupied electronic structure of this superstructure by spin- and angle-resolved inverse photoemission. The experimental results are accompanied by DFT calculations. We observe surface states and an image-potential resonance located several Å in front of the surface. Surprisingly, one surface state exhibits almost no Rashba splitting even though it is located around the Tl atoms. This result is explained by the orbital symmetry of the respective state. For the image resonance, we find hybridization with a downward dispersing TI state leading to spin-dependent spectral intensities that vary strongly close to the hybridization point. This observation, both in experiment and bandstructure calculations, is supported by charge distribution calculations showing an expeditious change from the image resonance to the TI-induced surface state depending on k_{||}.

[1] C. R. Ast *et al.*, Phys. Rev. Lett. **98**, 186807 (2007)

[2] G. Bihlmayer, S. Blügel, and E. V. Chulkov, Phys. Rev. B **75**, 195414 (2007)

[3] S. Wissing *et al.*, Phys. Rev. Lett. **113**, 116402 (2014)

[4] L. El-Kareh *et al.*, New J. Phys. **16**, 045017 (2014)

[5] P. Härtl, S. Schemmelm⁴, P. Krüger, M. Donath, and M. Bode, submitted to Phys. Rev. B

¹ Falicov Student Award Finalist

² AVS Graduate Research Awardee

³ Falicov Student Award Finalist

⁴ Falicov Student Award Finalist

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5:20pm **MI+2D+TF-WeA-10 Distinct Tamm and Shockley Surface States on Re(0001) Mixed by Spin-Orbit Interaction – A Photoemission Study**, **Marcel Holtmann**, *P. Krüger*, University of Münster, Germany; *K. Miyamoto*, *T. Okuda*, HiSOR, Japan; *P. Grenz*, University of Münster, Germany; *K. Shimada*, HiSOR, Germany; *M. Donath*, University of Münster, Germany

Tamm and Shockley states, these two paradigmatic concepts are used to describe surface states not only in electronic systems but also in photonic and phononic crystals. The Re(0001) surface was found to host both types of electronic surface states in neighboring, but qualitatively different gaps [1]. Interestingly, spin-orbit interaction generates a double W-shaped energy vs k_{\parallel} dispersion by mixing both types of states and lifting their spin degeneracy. We employ a combination of spin- and angle-resolved photoemission, tight-binding model calculations, and density functional theory that accounts for the photoemission process to establish reliable criteria for distinguishing between the two types of surface states. Our approach leads to a coherent understanding of the mechanism of spin-orbit interaction in such a situation.

From a detailed investigation of the Re(0001) surface along the ΓM and ΓK high-symmetry directions [2], we obtain Rashba parameters of 0.32 and 0.34 eVÅ along the two respective directions. This indicates a slight warping of the surface state. Regarding the aforementioned state's spin polarization: at variance with theoretical predictions for a perfect hcp(0001) of rhenium [3], we do not find any out-of-plane spin polarization. This is attributed to monatomic steps of a real Re(0001) surface with alternating terminations, leading on average to an effective sixfold surface symmetry and vanishing net out-of-plane spin polarization.

[1] M. Holtmann *et al.*, Phys. Rev. B **105**, L241412 (2022)

[2] M. Holtmann *et al.*, Phys. Rev. B **107**, 165420 (2023)

[3] A. Urru and A. Dal Corso, Surf. Sci. **686**, 22 (2019)

5:40pm **MI+2D+TF-WeA-11 Coupling between Spin Order and Orbital Order in 2D-Superlattice Perovskite Film**, **Bin Hu**, University of Tennessee Knoxville

INVITED

The coupling between spin order and orbital order presents a fundamental request to develop advanced multifunctional materials. 2D-superlattice perovskite films, known as solution-processing semiconductors, possess strong orbital order within non-degenerate Rashba band structures under the concurrent influence of spin-orbital coupling and symmetry breaking. This provides a fundamental condition to dynamically couple spin order and orbital order through multiferroic interface design. Here, we combine ferroelectric 2D-superalattice perovskite ($4,4\text{-DFPD}_2\text{PbI}_4$) film and ferromagnetic cobalt (Co) film to form multiferroic perovskite/Co interface. By using this multiferroic interface design, we found that the circularly polarized orbitals with right and left handedness (s^+ and s^-) in Rashba band structures can selectively interact with spin-up and spin-down spin dipoles on the Co surface, leading to a mutually selectivity between spin order and orbital order. Particularly, this selective interaction between spin order and orbital order can enable spin-switchable phenomena towards developing emerging functionalities in these solution-processing hybrid metal halide perovskites. When the ferromagnetic spins on the Co surface are altered between positive and negative magnetic field directions ($+\mathbf{B}$ and $-\mathbf{B}$), the circularly polarized luminescence (CPL) in 2D-superlattice perovskite can be switched between s^+ and s^- polarizations, leading to spin-switchable phenomena at room temperature. More interestingly, our polarized neutron reflectometry (PNR) studies found that circularly polarized photoexcitation generates a static magnetization within 2D-superalattice perovskite film prepared on the Co surface. This presents an optically induced magnetization phenomenon. Essentially, this optically induced magnetization reveals a long-range coupling between the spin order on the Co surface and the orbital order within Rashba band structures in 2D-superlattice perovskite film. This presentation will discuss the fundamental coupling between spin order and orbital order through Rashba band structures in 2D-superlattice perovskite film.

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