

O 70: Poster Wednesday: Electronic Structure

Time: Wednesday 17:45–20:00

Location: Poster B2

O 70.1 Wed 17:45 Poster B2

Predicting Dirac semimetals based on Sodium Ternary Compounds — ●BO PENG — Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — Department of Optical Science and Engineering and Key Laboratory of Micro and Nano Photonic Structures (Ministry of Education), Fudan University, Shanghai 200433, China. — TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom.

Predicting new Dirac semimetals, as well as other topological materials, is challenging since the relationship between crystal structure, atoms and band topology is complex and elusive. Here, we demonstrate an approach to design Dirac semimetals via exploring chemical degree of freedom. Based on understanding of the well-known Dirac semimetal, Na₃Bi, three compounds in one family, namely Na₂MgSn, Na₂MgPb and Na₂CdSn, are located. Furthermore, hybrid-functional calculations with improved accuracy for estimation of band inversion show that Na₂MgPb and Na₂CdSn have the band topology of Dirac semimetals. The nontrivial surface states with Fermi arcs on the (100) and (010) surfaces are shown to connect the projection of bulk Dirac nodes. Most importantly, the candidate compounds are dynamically stable and have been experimentally synthesized. The ideas in this work could stimulate further predictions of topological materials based on understanding of existing ones.

O 70.2 Wed 17:45 Poster B2

Resolving the electronic surface structure of Lanthanum Hexaboride (001) — ●PHILIPP BUCHSTEINER¹, FLORIAN SOHN^{2,3}, JAN VOIGT¹, GEETHA BALAKRISHNAN⁴, PETER BLÖCHL^{3,2}, and MARTIN WENDEROTH¹ — ¹IV. Physikalisches Institut, Georg-August Universität Göttingen, 37077 Göttingen, Germany — ²Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — ³Institut für theoretische Physik, Technische Universität Clausthal, 38678 Clausthal-Zellerfeld, Germany — ⁴Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

As Lanthanum Hexaboride (LaB₆) is a wide-spread cathode material for electron emitters, its surface has been studied for a long time [1]. While Scanning Tunneling Microscopy (STM) has shown up to now a (1x1) reconstructed surface [2], only recently a (2x1) reconstruction has been predicted by theory to be the most stable (001)-surface structure [3]. Using UHV low-temperature STM and Scanning Tunneling Spectroscopy (STS) we have investigated the LaB₆ (001) cleavage-plane. Our results confirm that atomically ordered surface areas are mostly labyrinth-like (2x1)-reconstructed. Combining STS and slab calculations within the framework of Density Functional Theory (DFT) allows us to further clarify the electronic structure, which is governed by 2p_z-orbitals of the boron octahedra. This work is supported by the DFG grant WE1889/10-1 and PR298/19-1. [1] M. Trenary, *Sci. Technol. Adv. Mater.*, 13 (2012) [2] J.S. Ozcomert, M. Trenary, *Surf. Sci.*, 265 (1992) [3] K. M. Schmidt et al., *Acta Mater.* 144, 187-201 (2018)

O 70.3 Wed 17:45 Poster B2

Orbital surface reconstruction on SrTiO₃ studied with resonant x-ray reflectometry — ●BENJAMIN KATTER¹, VOLODYMYR ZABOLOTNYI¹, EUGEN WESCHKE², LENNART DUDY¹, OZAN KIRILMAZ¹, SEBASTIAN MACKE³, MICHAEL SING¹, RALPH CLAESSEN¹, ROBERT GREEN⁴, and VLADIMIR HINKOV¹ — ¹Experimentelle Physik IV, Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany — ²BESSY II, Helmholtz-Zentrum Berlin for Materials and Energy, 12489 Berlin, Germany — ³Max Planck Institute for Metals Research, Heisenbergstraße 3, 70569 Stuttgart, Germany — ⁴Department of Physics & Astronomy, University of British Columbia, Vancouver, B.C. V6T 1Z1, Canada

Transition metal oxides, like all crystalline solids, can show reconstruction effects at their surface due to breaking of the crystal symmetry. In titanium terminated SrTiO₃, in which the surface symmetry is lowered from O_h to D_{4h} , we observe a lifting of orbital degeneracy and shifting of orbital energies of Ti at the surface. To explore this, we have used Resonant X-ray reflectometry (RXR) to analyze orbital reconstruction at the surface of SrTiO₃ by combining surface and bulk sensitive reflectometry scans. We found a reconstructed surface layer

of up to two unit cells in size where the optical constants of Ti were anisotropic. We fit and explain our results using crystal field theory.

O 70.4 Wed 17:45 Poster B2

Investigation of the electronic structure of triple-cations mixed-halides perovskites solar cell — ●SEBASTIAN LINKE — Helmholtz-Zentrum Berlin, Berlin, Germany — Humboldt Universität zu Berlin, Berlin, Germany

In the past years perovskite solar cells have attracted a lot of attention with conversion efficiencies exceeding 22%[1]. One of the most promising perovskite materials is the mixed halides triple cations perovskites, which are used in some of the most efficient perovskite solar cells. In the inverted structure the backcontact is usually formed by PTAA layer on top of ITO substrates. The physical processes however are not fully understood yet. In particular, the interfacial energy level alignments are not addressed.

In this work, photoelectron spectroscopy (PES) is used to investigate the electronic structure of the individual layers, i.e. the PTAA and perovskite, separately. Then, the energy level alignment when forming the interfaces will be investigated, providing the information on the energy barrier of the charge carriers.

[1]Green et al.; Solar cell efficiency tables (version 52).; *Prog Photovolt Res Appl.* 2018;26:427*436.; <https://doi.org/10.1002/pip.3040>

O 70.5 Wed 17:45 Poster B2

Scanning Tunneling Spectroscopy on the f-electron system Praseodymium Hexaboride — ●LISA HARMSSEN¹, PHILIPP BUCHSTEINER¹, GEETHA BALAKRISHNAN², and MARTIN WENDEROTH¹ — ¹IV. Physikalisches Institut, Georg-August Universität Göttingen, 37077 Göttingen, Germany — ²Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

The surfaces of f-electron systems like rare-earth hexaborides are prone to host correlation effects, such as heavy Dirac fermions [1]. While the Samarium Hexaboride surface have been studied in the past [2], only little is known about the electronic surface structure of the neighbouring f-electron system Praseodymium Hexaboride (PrB₆). Here, we have investigated the (001)-cleavage plane of PrB₆ with Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) down to 8 K. The acquired data reveals non reconstructed areas as well as several surface reconstructions. In contrast to Photoemission Spectroscopy measurements [3], where a large surface area is mapped, we are able to resolve the electronic structure locally including the local structure as seen in constant current topographies. This opens a way to disentangle f-electron physics on the atomic scale. This work is supported by the DFG grant WE1889/10-1 and PR298/19-1. [1] H. Pirie et al., *arXiv:1810.13419 [cond-mat.str-el]* (2018) [2] S. Rößler et al., *Philos. Mag.*, 96:31, 3262-3273 (2016) [3] S. Patil et al., *J. Phys.: Condens. Matter* 23, 495601 (2011)

O 70.6 Wed 17:45 Poster B2

Experimental Growth and Characterization of Bi:CeAg_x/Ag(111) — ●HENDRIK BOSTELMANN-ARP, KATHARINA KISSNER, CHUL-HEE MIN, and FRIEDRICH REINERT — Julius Maximilians University of Würzburg, 97074 Würzburg

Recent theoretical studies point towards a new class of topologically non trivial materials, where the interplay of electronic correlation and strong spin orbit coupling is the driving force [1, 2]. Nevertheless, the existence of topological features in correlated systems has never been unambiguously clarified. Therefore, a first goal must be to realize materials in which both effects, spin orbit coupling and strong correlation, are observable. Very recently the influence of spin orbit coupling was reported in the substitution series Ce₃Bi₄(Pt_{1-x}Pd_x) (0 ≤ x ≤ 1), where the replacement of the heavier element Pt with the lighter Pd is suggested to induce a Kondo insulator to semimetal transition [3]. In this contribution we propose to merge electronic correlation and strong spin orbit coupling in the epitaxially grown surface alloy Bi:CeAg_x on Ag(111). The surface lattice symmetry is determined by means of Low Energy Electron Diffraction. Furthermore, we investigate the changes in electronic dispersion as well as Ce 3d core level structure by Angle Resolved and X-Ray Photoelectron Spectroscopy. [1] M. Dzero, et al., *Phys. Rev. Lett.* 104, 106408 (2010) [2] J. Allen, *Phil. Mag.* 96, 3227 (2016) [3] S. Dzaber, et al., *Phys. Rev. Lett.* 118, 246601 (2017)

O 70.7 Wed 17:45 Poster B2

Fermi-Löwdin orbital self-interaction corrected DFT: application to phenolic acids — ●JAKOB KRAUS, SEBASTIAN SCHWALBE, TORSTEN HAHN, and JENS KORTUS — TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany

The Fermi-Löwdin orbital self-interaction correction (FLO-SIC)[1] aims to counter the well-known self-interaction error (SIE) of density functional theory (DFT) in a computationally efficient and size-extensive way. FLO-SIC has been shown to reproduce the correct $-1/r$ behavior of the potential as well as an adequate binding energy curve for stretched-bonds systems, a clear improvement over uncorrected DFT [2]. For selected phenolic acids, namely gallic acid and some of its derivatives, the bond-dissociation enthalpies (BDEs) as well as the ionization potentials (IPs) have been evaluated in the gas phase and in several test solvents. These molecular properties will be useful to predict a reaction path for the well-documented antioxidant properties of phenolic acids [3]. All results are presented as a comparison between uncorrected DFT and the most recent implementation of FLO-SIC DFT.

[1] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)

[2] S. Schwalbe et al., J. Comput. Chem., vol. 39, 2463 (2018)

[3] M. Nsangou et al., J. Mol. Struct., vol. 850, 135 (2008)

O 70.8 Wed 17:45 Poster B2

Vipster – A novel editor and visualization tool for periodic structures — ●SEBASTIAN GSÄNGER, JONATHAN GRUBER, and BERND MEYER — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

When preparing structures for atomistic simulations or analyzing their results, one often has to decide between editing and visualization software. This is even more prevalent when dealing with periodic calculations, for which support has often been added to established programs as an afterthought. Here we present our endeavor to fill this gap with a portable and self-contained package that handles periodicity as a primary property. Utilizing modern platform-independent technology, we provide a featureful desktop client for all major operating systems, as well as a lightweight browser-based client and a scripting-interface via python.

O 70.9 Wed 17:45 Poster B2

PyFLOSIC: OpenSource implementation of Fermi-Löwdin orbital self-interaction corrected DFT — ●SEBASTIAN SCHWALBE¹, LENZ FIEDLER¹, KAI TREPTE², TORSTEN HAHN¹, and JENS KORTUS¹

— ¹TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany — ²Central Michigan University, Department of Physics, USA

We present the first developer version of the OpenSource implementation of the Fermi-Löwdin orbital self-interaction correction (FLO-SIC) [1,2] within the highly modular and modern PySCF code infrastructure. FLO-SIC aims to counter the well-known self-interaction error (SIE) of density functional theory (DFT) in a computationally efficient and size-extensive way, replacing the explicit solution of the N^2 localization equations with the optimization of $3N$ so called Fermi-orbital descriptors. The new implementation allows the usage of different unified Hamiltonians and is written in density matrix notation. These methodical changes allow the FLO-SIC method to be applicable on any functional implemented in the libxc library. Various examples for FLO-SIC applied to LDA-PW, the GGA functional PBE as well as the promising metaGGA SCAN functional will be discussed in detail.

[1] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)

[2] S. Schwalbe et al., J. Comput. Chem., vol. 39, 2463 (2018)

O 70.10 Wed 17:45 Poster B2

Proton uptake in the mixed ionic and electronic conductor BaFeO_{3-x} — ●MAXIMILIAN F. HOEDL, ROTRAUT MERKLE, EUGENE A. KOTOMIN, and JOACHIM MAIER — Max Planck Institute for Solid State Research, Stuttgart, Germany

Many solid oxides containing oxygen vacancies can dissociatively absorb water leading to mobile protonic defects (hydroxide ions on oxide ion sites) in the lattice. The magnitude of water uptake appears to be determined by the basicity of the oxide ions in the solid. However, recent experimental studies suggest that in ionic-electronic mixed conductors such as BaFeO_{3-x} perovskites, the water uptake can be disfavored by an interaction between protons and electron holes.[1] We present the results of first-principles DFT+U and HSE06 calculations on the interplay between the complex electronic structure and the water uptake in BaFeO_{3-x}. The strong correlation effects of Fe3d electrons lead to a significant energy separation of spin-up and spin-down sub-bands. The spin-up band eventually falls below the O2p states and thus triggers a negative charge transfer from the oxide ions to the iron ions, creating holes in the O2p valence band. This reduces the negative charge on the oxide ions and the oxide ion basicity. The calculated hydration enthalpies depend on the hole concentration varying between zero for BaFeO₃ and about -1 eV for BaFeO_{2.6}. [1] R. Zohourian et al., Adv. Funct. Mater. 2018, 28, 1801241