O 62: Poster Wednesday: Topology and Symmetry-Protected Materials

Time: Wednesday 17:45–20:00 Location: Poster B1

O 62.1 Wed 17:45 Poster B1

Probing topological superconductivity in Indium doped topological crystalline insulator using high resolution photoemission spectroscopy — •Sangeeta Thakur[1,2,4], Deepnarayan Biswas[1], Akansha Singh[3], Pransjit Sen[3], K. Srinivas[1], A. Thamizhavel[1], Giovanni Di Santo[2], L. Petaccia[2], and K. Maiti[1] — [1]Tata Institute of Fundamental Research Colaba Mumbai India — [2]Elettra Sincrotrone Trieste, Trieste, Italy — [3]Harsh-Chandra Research Institute, HBNI, Allahabad, India — [4]Freie Universität Berlin, Institut für Experimentalphysik, Berlin, Germany

Pb0.6Sn0.36In0.04Te single crystals were investigated by high resolution photoemission spectroscopy to probe the topological superconductivity predicted for indium doped topological crystalline insulator (TCI). XRD measurements on Pb0.6Sn0.36In0.04Te confirm the rock-salt structure peculiar for TCI. Angle resolved photoemission spectra show the signature of Dirac cone surface states which gives evidence for an inverted band structure as in the pristine Pb0.6Sn0.36Te TCI sample. The experimental valence band spectra can be explained reasonably well by the theoretical calculations. Presence of topological surface state makes Pb0.6Sn0.36In0.04Te a potential material to find the topological superconductivity in TCI.

O 62.2 Wed 17:45 Poster B1

Study of ARPES, Magnetic and magneto-transport properties of Dy doped Bi2Te3 Topological Insulator — •Vinod Kumar Gangwar[1], Shiv Kumar[2], Yufeng Zhang[3], Prashant Shahi[4], Swapnil Patil[1], Eike Fabian Schwier[2], Kenya Shimada[2], Yoshiya Uwatoko[3], and Sandip Chatterjee[1] — [1]Department of Physics, Indian Institute of Technology (BHU) Varanasi 221005 — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima City, 739-0046 Japan — [3]Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan — [4]Department of Physics, D.D.U. Gorakhpur University, Gorakhpur 273009

Topological insulators are characterized by a gapped bulk state and gapless surface or edge states that is protected by time-reversal symmetry (TRS). TRS can be broken by magnetic impurities. To investigate the correlation between topological state and magnetism it is important to introduce magnetic elements into Topological insulators. In this study, we have synthesized the single crystals of Bi2-xDyxTe3 (x =0.06, 0.10, 0.16) and reported the effects of Dysprosium substitution on the topological properties in Bi2-xDyxTe3. XRD data indicate very good single crystallinity of Bi2-xDyxTe3 without any sign of secondary phase. We have measured the magnetization M(H) at different temperature and found that at low temperature it shows weak ferromagnetic ordering. From the ARPES and thermoelectric studies we found n-type nature of Dy doped Bi2Te3.

O 62.3 Wed 17:45 Poster B1

Theoretical study of the candidate material for type-II Weyl semimetal $MoTe_2$ using relativistic KKR method — •Ryota Ono[1], Yoshitaka Nakata[1], Alberto Marmodoro[2], Jan Minár[3], Hubert Ebert[2], Kazuyuki Sakamoto[4], and Peter Krüger[4] — [1]Department of Materials Science (Frontier Science Program), Graduate School of Science and Engineering, Chiba University, Chiba 263-8522, Japan — [2]Department of Chemistry, University of Munich, Butenandstr. 5-13, D-81377 München, Germany — [3]University of West Bohemia, New Technologies - Research Center, Univerzitni 8, 306 14 Plzeň, Czech Republic — [4]Graduate School of Science and Engineering and Molecular Chirality Research Center, Chiba University, Chiba 263-8522, Japan

Topological Weyl semimetals (TWS) are examples of Dirac materials, in which relativistic and quantum mechanical effects give rise to new physical features such as chiral anomaly in the transport of charged particles, giant anomalous Hall effect and emergence of Weyl fermions. TWSs can be classified into type-I and type-II according to whether they respect Lorenz invariance. $MoTe_2$ is a transition metal dichalcogenide (TMDC) and forms many phases, among which the T_d phase has been proposed as a candidate material for a type-II Weyl semimetal. Here we calculated the electronic structure of T_d $MoTe_2$ and explored its band structure around a Weyl point. Using the spin polarized relativistic KKR method, we also calculated ARPES in the one-step model which takes into account all matrix, surface and final state photoemission effects. The results are compared with experiment.

O 62.4 Wed 17:45 Poster B1

Type-II Weyl semimetals – spin-polarization, impurity scattering, and a polar instability — •Philipp Rüssmann[1], Phivos Mavropoulos[1,2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Department of Physics, National and Kapodistrian University of Athens, 15784 Zografou, Greece

Weyl semimetals are a new class of materials that host topologically protected crossings in their bulk electronic structure. Their intriguing transport properties have the potential to spark the development of radically new technologies based on topological semimetals. However, to fully realise their potential in the future, a microscopic understanding of the topological phase is required in terms of their nature of the phase transition and the functional response to impurities. In recent joint studies [1,2] we investigated the type-II Weyl semimetal candidates $MoTe_2$ and WTe_2 by combining DFT calculations with STM and ARPES experiments. Here, focusing on the theoretical side, we discuss evidence of a polar instability near the structural phase transition from the topologically trivial to the non-trivial Weyl phase in $MoTe_2$ [1]. In studying the response of both surface and bulk states to perturbations in topologically trivial WTe_2 and the stable Weyl phase in $MoTe_2$, we are able to uncover the existence of a universal response of surface- and bulk-derived topologically protected quasiparticles to naturally occurring defects in the crystals [2].

[1] A. P. Weber, *et al.* PRL **121**, 156401 (2018)
[2] P. Rüßmann, *et al.* PRB **97**, 075106 (2018)

O 62.5 Wed 17:45 Poster B1

Bulk band structure of Sb_2Te_3 — •Henriette Elisabeth Lund[1], Ann Julie Utne Holt[1], Martin Bremholm[2], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark — [2]Department of Chemistry and iNANO, Aarhus University, 8000 Aarhus C, Denmark

Sb_2Te_3 belongs to the class of materials known as topological insulators. The surface electronic structure of the material has been investigated with both angle-resolved photoemission spectroscopy (ARPES) and spin-resolved ARPES, but little is known about the bulk electronic structure of the material.

In the present study, the bulk and surface electronic structure of Sb_2Te_3 is investigated by means of ARPES performed at the ASTRID 2 synchrotron radiation facility in Aarhus, Denmark. The ARPES experiments reveal the presence of both two-dimensional and three-dimensional states in the band structure. The three-dimensional band structure is determined along high-symmetry directions in the Brillouin zone and compared to published band structure calculations.

O 62.6 Wed 17:45 Poster B1

Surface Berry curvature dipole in topological materials — •Dennis Wawrzik[1], Jhih-Shih You[1], Inti Sodemann[2], and Jeroen van den Brink[1,3] — [1]Institute for Theoretical Physics, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzerstr. 38, 01187 Dresden, Germany — [3]Department of Physics, Technical University Dresden, Helmholtzstr. 10, 01062 Dresden, Germany

Recently the research on understanding the effects of quantum geometry in novel materials has attracted considerable attentions both in theory and in experiment. A remarkable example is the Hall-like current that can occur in second-order response to an external electric field in materials with time-reversal symmetry but broken inversion symmetry, as a result of the dipole moment of the Berry curvature (BCD). However, the BCD is not allowed if a bulk has high crystalline symmetries. We show that for a proper chosen surface breaking some of these bulk symmetries one can find a non-vanishing surface BCD. The proposed effect could be observed in topological materials with a conducting surface like Weyl semimetals and TCIs.

O 62.7 Wed 17:45 Poster B1

Topological surface states in semi-metallic Tm monochalcogenides — •Chul-Hee Min[1], Chang Jong Kang[2], Katharina Kissner[1], Hendrik Bentmann[1], Dong-Choon Ryu[3], Woo Jae Choi[4], Yong-Seong Kwon[4], Volodymyr Zabolotnyy[1], Vladimir Hinkov[1], Byung-Il Min[3], and Friedrich Reinert[1] — [1]Universität Würzburg, EP7, Würzburg, Germany — [2]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08856, USA — [3]Department of Physics, PCTP, POSTECH, Pohang 37673, Korea — [4]Department of Emerging Materials Science, DGIST, Daegu 42988, Republic of Korea

Topological surface states with strongly localized 4f character have not been clearly identified in experiments yet. Analogous to hypothetically topological non-insulating rare earth materials, e.g. g-SmS and SmO [1,2], we propose Thulium monochalcogenides, $TmSe_{1-x}Te_x$, to be a very promising candidate to realize even topological Dirac or Weyl semimetals. The compounds having simple fcc structure show mixed valency overall, and insulating behaviors in resistivity. By means of ARPES, their Fermi surface maps and constant energy cuts will be present, which show a good agreement with our DFT calculation results. If the energy positions of 4f bands of Tm in DFT results can be renormalized with factor of 0.1, we can identify most of theoretical Fermi surface features, including the $4f$ surface states.

[1] D. Kasinathan, K. Koepernik, L. H. Tjeng, and M. Haverkort, Phys. Rev. B, 91 195127 (2015). [2] C.-J. Kang, H.-C. Choi, Kyoo Kim, and B. I. Min, Phys. Rev. Lett., 114, 166404 (2015).

O 62.8 Wed 17:45 Poster B1

Anomalous behavior of the electronic structure of $(Bi_{1-x}In_x)_2Se_3$ across the quantum-phase transition from topological to trivial insulator — •Friedrich Freyse[1], Irene Aguilera[2], Lada Yashina[3], Daria Tsukanova[3], Alexander Chaika[4], Carolien Callaert[5], Artem Abakumov[6], Joke Hadermann[5], Andrei Varykhalov[1], Emile Rienks[1], Gustav Bihlmayer[2], Stefan Blügel[2], Oliver Rader[1], and Jaime Sánchez-Barriga[1] — [1]Helmholtz-Zentrum Berlin — [2]Forschungszentrum Jülich and JARA — [3]Moscow State University — [4]Institute of Solid State Physics RAS — [5]University of Antwerp — [6]Skolkovo Institute of Science and Technology

Using spin- and angle-resolved photoemission and relativistic many-body calculations, we investigate the electronic structure of topological surface states (TSSs) across a topological quantum-phase transition in $(Bi_{1-x}In_x)_2Se_3$ bulk single crystals. By increasing x, we observe how a surface gap opens at the Dirac point of the initially gapless TSS of Bi_2Se_3, leading to the existence of massive fermions with non-zero spin polarization. The surface gap monotonically increases for a wide range of x values in both the topological and trivial sides of the phase transition. Our calculations reveal qualitative agreement with the experimental results all across the quantum-phase transition upon the systematic variation of the spin-orbit coupling strength. A non-time-reversal symmetry-breaking mechanism of bulk-mediated scattering processes that increase with decreasing spin-orbit coupling strength is proposed as explanation.