Topological Weyl Semimetals

Binghai Yan, Chandra Shekhar, Yan Sun, Shu-Chun Wu, Nitesh Kumar, Vicky Süβ, Claudia Felser*

In the frontier of condensed-matter physics, the Weyl semimetals (WSMs) are the new star materials. The WSM is a semimetal regarded as the 3D analogue of graphene, wherein the electronic bands linearly disperse around pairs of nodes, the Weyl points, of fixed (left or right) chirality. We, an interdisciplinary team of our institute, have been carrying out pioneering experimental research on WSM materials (Nb,Ta)(P,As) with the guidance of theoretical calculations. For the first time, we report giant, positive magnetoresistance (MR), which are larger than those of all known materials, and ultrahigh mobility in NbP [1]. We also explore the exotic negative MR in these WSM compounds[2], aiming to long-sought chiral anomaly effect. Further, we reveal the topological Fermi arcs on WSM surfaces [3,4] in collaboration with the ARPES collaborators. Our work holds promise for foreseeable applications such as valleytronics and spintronics.

We conduct interdisciplinary research covering solid state chemistry, quantum magneto-transport ARPES and condensed-matter theory, which involves active young researchers from three divisions inside our institute (solid state chemistry, chemical metals science, physics of quantum materials) and close external collaborators from Dresden (MPI PKS, HLD-EMFL), Netherlands (HFML-EMFL) and United Kingdom (Oxford).

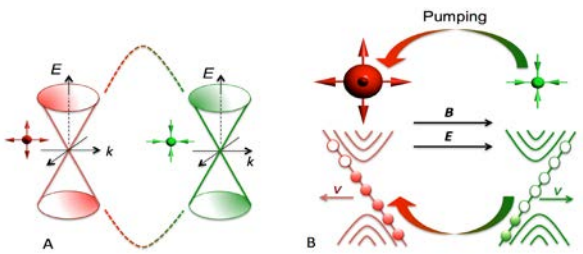

Fig.1 Illustration of Weyl points with opposite chirality and the chiral anomaly effect by charge pumping between two Weyl points.

In a WSM, the Weyl point acts as a monopole with fixed chirality in the momentum space and promises the realization of an exotic quantum phenomenon: the chiral anomaly, which is expected to induce unconventional negative longitudinal MR = $\Delta R(B)/R(0)$ (magnetic field B $\parallel$ current I) in WSMs. The chiral anomaly effect (chiral symmetry breaking) has been sought for decades in high-energy physics after the prediction in 1969, which is regarded as important as a fundamental law. If it is successfully realized by the Weyl fermion quasipaticles, the chiral anomaly will connect the condensed-matter physics and high-energy physics as a new bridge. On the surface, topological Fermi arcs (unclosed Fermi surfaces) between two Weyl points with opposite chirality is another important manifestation of the non-trivial topological nature of WSMs.

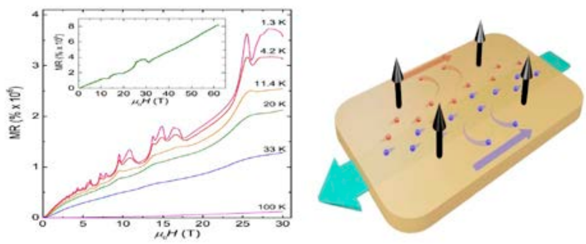

Fig. 2 Giant positive MR observed in NbP and the schematics of large MR induced by coexistence of electron and hole carriers.

Giant positive transverse MR. In the search of negative MR, surprisingly we observed giant positive transverse MR (B$\perp$I) in the WSM material NbP for the first time [1]. With the high-quality single crystal samples synthesized (Dr. Marcus Schmidt), an extremely large MR of 3.6×10^6 % at 1.3 K and 30 T and even 8.1×10^6 % at 62 T and 1.5 K was discovered (Dr. Chandra Shekhar), in collaboration with high magnetic field labs in Dresden (HLD-EMFL, Prof. Jochen Wosnitza) and Netherlands (HFML-EMFL, Prof. Uli Zeitler). Meanwhile very high mobility was observed, which we attributed to the linear band structure that exhibits high Fermi velocity and the robustness against back-scattering due to the Berry phase. Besides the Weyl points, NbP exhibits normal electron and hole pockets in the band structure like a normal semimetal, in which the electron-hole resonance usually induces large positive MR. Hence, NbP presents a unique example of a material combining topological and conventional electronic phases, with intriguing physical properties resulting from their interplay. The recognized giant MR was previously only known to occur in some complexly structured materials. NbP or a material with similar properties could now offer an alternative for significantly easier designs of future MR devices. This work was extensively reported by scientific medias as soon as it was publish online in Nature Physics [1].

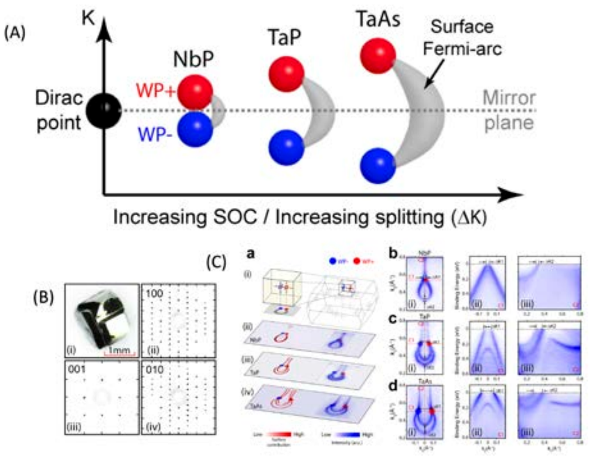

Fig. 3 (A) Illustration of the separation of a pair of Weyl points (with opposite chirality, marked as WP+ and WP-) controlled by the SOC strength of different compounds of the family. (B) Image of NbP single crystals with shining flat surface used for ARPES measurements. and X-ray diffraction patterns. (C) Calculated (red) and measured Fermi arcs for NbP, TaP and TaAs.

Topological Fermi arcs. Based on our high quality single crystals, our close collaborator Prof. Yu-Lin Chen in Oxford observed clearly Fermi arcs on the surface of TaAs [3], NbP, TaP and NbAs [4] by ARPES, which is supported by our accurate *ab initio* calculations [3-5]. By systematically investigating NbP, TaP and TaAs from the same transition metal monopnictide family, we discovered their Fermiology evolution with SOC strength, revealing the mechanism to realize and fine-tune the electronic structures of WSMs. Based on accurate *ab-initio* simulations [5], we further predicted the spin-textures and the Lifshitz-transition of the Fermi surfaces by materials engineering, which has been verified by recent ARPES measurements []. The discovery of this family of WSMs provides a rich material base for exploring many exotic physical phenomena and novel future applications.

Future directions. (i) We have successfully verified the topological nature of the WSM compounds in both theoretical calculations and ARPES experiments. So we can further look for the chiral anomaly effect based on these materials. In the transport measurement of TaP, we have achieved important indications of the negative MR recently [2]. (ii) The WSM carries giant Berry curvatures in the momentum space near the Fermi energy, because its conduction and valence bands cross linearly through nodes that are singularity points (source/sink) of the Berry curvature. Considering the large Berry curvatures and strong spin-orbit coupling in a WSM, we propose that a WSM can exhibit a strong intrinsic spin Hall effect (SHE), which is a manifestation of the spin-dependent Berry phase. The SHE can be used to electrically generate or detect spin currents in spintronic devices. These spin currents can, in particular, be used to excite or manipulate magnetic nano-elements and domain walls. In collaboration with Prof. Stuart Parkin in MPI Halle, we will perform both theoretical and experimental investigations of the SHE of the WSM TaP and related compounds that have been discovered recently. Our proposed SHE devices will pave the way to room-temperature applications of topological materials.

References

[1] *C. Shekhar, A. K. Nayak, Y. Sun, M. Schmidt, M. Nicklas, I. Leermakers, U. Zeitler, Y. Skourski, J. Wosnitza, Z.K. Liu, Y.L. Chen, W. Schnelle, H. Borrmann, Y. Grin, C. Felser, and B. Yan, Nature Physics 11, 645–649 (2015) DOI:10.1038/NPHYS3372.*

[2] *C. Shekhar, F. Arnold, S.-C. Wu, Y. Sun, M. Schmidt, N. Kumar, A. G. Grushin, J. H. Bardarson, R. D. D. Reis, M. Naumann, M. Baenitz, H. Borrmann, M. Nicklas, E. Hassinger, C. Felser, and B. Yan, arXiv:1506.06577 (2015).*

[3] *L. X. Yang, Z. K. Liu, Y. Sun, H. Peng, H. F. Yang, T. Zhang, B. Zhou, Y. Zhang, Y. F. Guo, M. Rahn, P. Dharmalingam, Z. Hussain, S. K. Mo, C Felser, B. Yan, and Y. L. Chen, Nature Physics 11, 728 (2015). DOI: 10.1038/NPHYS3425.*

[4] *Z. K. Liu, L. X. Yang, Y. Sun, T. Zhang, H. Peng, H. F. Yang, C. Chen, Y. Zhang, Y. F. Guo, P. Dharmalingam, M. Schmidt, Z. Hussain, C. Felser, S. K. Mo, B. Yan, and Y. L. Chen, Nature Materials (2015) DOI:10.1038/NMAT4457.*

[5] *Y. Sun, S.-C. Wu, B. Yan, Phys. Rev. B,* ***92****, 115428 (2015).*

* Binghai.Yan@cpfs.mpg.de