

Inverted band structure of topological Dirac-semimetal candidate CaAuAs

Kosuke Nakayama,^{1,2} Zhiwei Wang,³ Daichi Takane,¹ Seigo Souma,^{4,5*} Yuya Kobota,¹ Miho Kitamura,⁶ Koji Horiba,⁶ Hiroshi Kumigashira,^{6,7} Takashi Takahashi,^{1,4,5} Yoichi Ando,³ and Takafumi Sato^{1,4,5}

¹ Department of Physics, Tohoku University, Sendai 980-8578, Japan

² PRESTO-JST, Tokyo 102-0076, Japan

³ Institute of Physics II, University of Cologne, Köln 50937, Germany

⁴ Center for Spintronics Research Network, Tohoku University, Sendai 980-8577, Japan

⁵ WPI-AIMR, Tohoku University, Sendai 980-8577, Japan

⁶ Photon Factory, Institute of Materials Structure Science, High Energy Research Organization, 1-1 Oho, Tsukuba, 305-0801, Japan

⁷ IMRAM, Tohoku University, Sendai 980-8577, Japan

1 Introduction

Topological Dirac semimetals (TDSs), a three-dimensional analogue of graphene, are attracting particular attentions since they are a useful platform to study an intriguing quantum physics triggered by three-dimensional Dirac fermions. Recent first-principles band-structure calculations have predicted that CaAuAs possesses a pair of Dirac cones close to the Fermi level (E_F) along the ΓA line of the bulk Brillouin zone (BZ) due to the bulk-band inversion and the protection by the C_3 symmetry [1]. The predicted simple band structure with no E_F crossings of other topologically trivial bands makes CaAuAs an ideal system to search for exotic properties associated with bulk Dirac fermions. To examine possible 3D-TDS nature of CaAuAs, we have performed soft x-ray ARPES to reveal the electronic structure relevant to 3D Dirac fermions and clarify its possible link to the exotic physical properties [2].

2 Experiment

High-quality single crystals of CaAuAs were grown by the self-flux method. Angle-resolved photoemission spectroscopy (ARPES) measurements were performed with a SES2002 electron analyzer at BL2. We used linearly polarized light of 300-600 eV. The energy and angular resolutions were set to be 150 meV and 0.2° , respectively. Crystals were cleaved *in situ* in an ultrahigh vacuum better than 1×10^{-10} Torr along the (0001) crystal plane. Sample temperature was kept at $T = 40$ K during the ARPES measurements.

3 Results and Discussion

By utilizing bulk-sensitive soft-x-ray photons from synchrotron radiation, we experimentally determined the bulk valence-band structure in the 3D bulk BZ of CaAuAs, and found a semimetallic band overlap between holelike As 4*p* and electron-like Au 6*p* bands. As schematically shown in Fig. 1(a), our ARPES measurements revealed that the Fermi surface (FS) of CaAuAs consists of 3D electronlike (e_1) and holelike (h_1) pockets centered at the Γ and A points, respectively, as well as a quasi-2D holelike (h_2) cylinder along the ΓA line. The formation of a quasi-2D cylindrical FS is probably associated with the hole

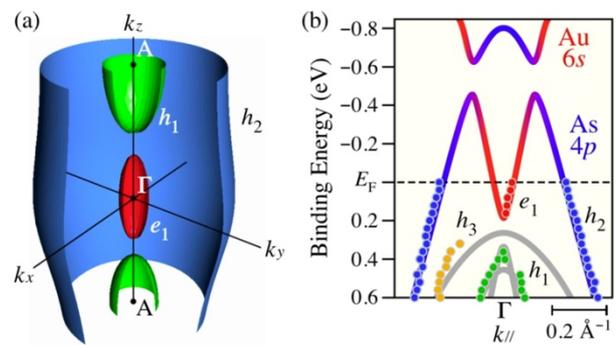


Fig. 1: (a) Schematic 3D view of the FS for CaAuAs deduced from the ARPES experiment. (b) Experimental band dispersion around the Γ point in $k_z=0$ plane, compared with the calculated band dispersion with spin-orbit coupling along the ΓM line (solid curves) [1].

doping to the crystal. After taking the hole doping into account, we found a good agreement between the experimental and calculated bulk bands. In particular, the band dispersion at $k_z = 0$ coincides nearly perfectly with the calculation in which the chemical potential is shifted downward by 300 meV [1]. The present result demonstrates that the bulk-band structure of CaAuAs is well captured by the band-structure calculations. Because of the high tunability in the chemical composition of this compound, CaAuAs provides a precious opportunity for exploring novel quantum phenomena associated with the Dirac fermions, and for investigating the novel properties of 3D Dirac quantum phase transition from TDS to other exotic topological phases.

Acknowledgement

We thank T. Kim, C. Cacho (Diamond Light Source), and S. A. Ekahana, M. Shi (Swiss Light Source) for their collaboration on this work.

References

- [1] B. Singh *et al.*, Phys. Rev. B **98**, 085122 (2018).
- [2] K. Nakayama *et al.*, Phys. Rev. B (R), *in press*.

* s.souma@arpes.phys.tohoku.ac.jp