ALS SCIENCE HIGHLIGHT

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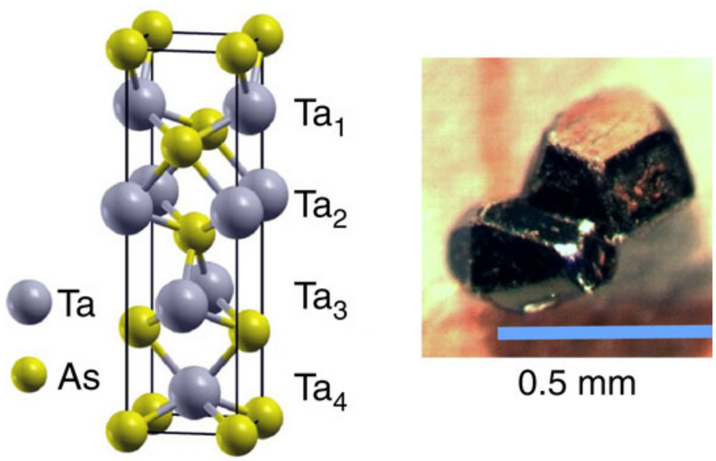
# Weyl Fermions Discovered After 85 Years

An international team led by Princeton University scientists has discovered an elusive massless particle first theorized 85 years ago: the Weyl fermion. It was detected as an emergent quasiparticle in synthetic crystals of the semimetal, tantalum arsenide (TaAs). Using angle-resolved photoemission spectroscopy (ARPES), the researchers studied the surface and bulk band structure of TaAs. The results exhibit the features—cones, nodes, and arcs—that establish the presence of Weyl fermions. These exotic particles, if applied to next-generation electronics, could allow for the nearly free and efficient flow of electricity, and thus greater power, in devices such as computers. More generally, the work paves the way for the realization of many fascinating topological quantum phenomena.




**Left: Crystal structure of TaAs, shown as stacked Ta and As layers. The lattice of TaAs does not exhibit space inversion symmetry. Right: Photo of TaAs single crystals.**

Weyl fermions were proposed by the mathematician and physicist Hermann Weyl in 1929 as an alternative to Einstein's theory of relativity. Although that application never panned out, the characteristics of his theoretical particle intrigued physicists for nearly a century. Unlike electrons, Weyl fermions are massless and possess a high degree of mobility. They also possess a form of chirality in which their spin is either in the same direction as motion (right-handed) or in the opposite direction (left-handed). Their basic nature means that Weyl fermions move very quickly on the surface of the crystal with no backscattering, which hinders efficiency and generates heat in normal electronic materials.

According to established theory, a Weyl semimetal state could only arise in a crystal where either time-reversal symmetry or inversion symmetry is broken. Initially, the team researched hundreds of crystal structures and simulated dozens of likely structures. They published an earlier paper theorizing that Weyl fermions could exist in a class of materials composed of a transition metal (e.g. Ta or Nb) and a Group 15 element (e.g. As or P). They synthesized asymmetrical TaAs crystals and brought them to the ALS (Beamlines 4.0.3, 10.0.1, and 12.0.1) as well as other synchrotron light sources (Stanford Synchrotron Radiation Lightsource, Diamond Light Source,

Publication about this research: S.-Y. Xu et al., "Discovery of a Weyl fermion semimetal and topological Fermi arcs," *Science* **349**, 6248 (2015); and S.-M. Huang et al., "A Weyl Fermion semimetal with surface Fermi arcs theoretically predicted in the transition metal monopnictide TaAs class," *Nat. Commun.* **6**, 7373 (2015).

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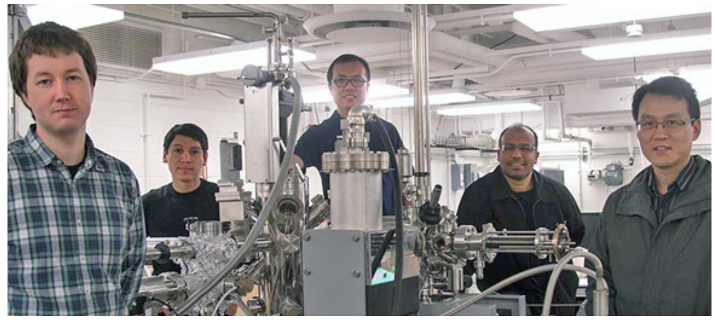
## Materials By Design

Stone, bronze, iron, silicon: in ages past and present, materials have had the power to shape civilization. Now, some believe we are on the verge of a golden age of materials science, in which new materials are rationally designed rather than discovered by accident or through painstaking trial and error. Converging advances in supercomputing, nanofabrication, and materials characterization (at facilities such as the ALS) are enabling new materials specifically designed for artificial photosynthesis, for example, or for processing more information in less space at lower power.

In this work, Xu et al. sifted through hundreds of materials with the desired structural characteristics, identified the ones likely to be semimetals or narrow-bandgap semiconductors, and performed systematic calculations of their band structures. "The nature of this research and how it emerged is really different and more exciting than most of other work we have done before," Xu said. "Usually, theorists tell us that some compound might show some new or interesting properties, then we as experimentalists grow that sample and perform experiments to test the prediction. In this case, we came up with the theoretical prediction ourselves and then performed the experiments. This makes the final success even more exciting and satisfying than before."



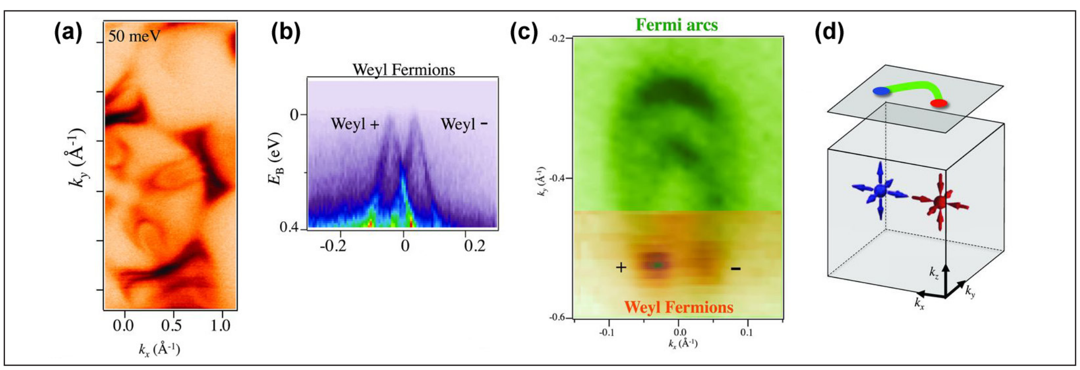
**Princeton team members (from left to right): Ilya Belopolski, Daniel Sanchez, Guang Bian, M. Zahid Hasan, and Hao Zheng. (Photo by Danielle Alio, Office of Communications.)**

and the Swiss Light Source) to perform ARPES experiments.

Using a combination of vacuum ultraviolet (VUV) and soft x-ray (SX) ARPES, the researchers systematically studied the surface and bulk electronic structure of TaAs. The surface-sensitive VUV-ARPES measurements demonstrated the existence of Fermi-arc surface states, consistent with earlier band calculations. The SX-ARPES measurements, which are reasonably bulk sensitive, revealed 3D (bulk) Weyl cones with linear dispersions, similar to the 2D (surface) Dirac cones associated with topological insulators and graphene. When the tips of the cones overlap slightly, there is no bandgap, and the material is considered a semimetal (insulators and semiconductors have bandgaps). When the tips meet at a single point, it is a Weyl semimetal, and the point is called a Weyl node.

Superimposing the SX-ARPES bulk data containing the Weyl nodes onto the VUV-ARPES data containing the surface Fermi arcs to scale, the researchers noted that all the arc terminations and projected Weyl nodes match within the experimental resolution. Because the SX-ARPES bulk data and the VUV-ARPES surface data are completely independent measurements obtained at two different beamlines, the fact that they match well provides another piece of evidence of the topological nature (the surface–bulk correspondence) of the Weyl semimetal state in TaAs.

Although practical technologies are still a long way off, publications about Weyl fermions have increased rapidly since the discovery was reported, signifying the opening of an exciting new frontier in condensed matter physics. "The physics of the Weyl fermion are so strange," said M. Zahid Hasan, the Princeton physics professor who led the research team, "there could be many things that arise from this particle that we're just not capable of imagining now."




**(a) ARPES Fermi-surface map showing horseshoe-shaped Fermi arcs. (b) ARPES bulk dispersion map showing two linearly dispersive Weyl cones. Plus and minus signs denote right- and left-handed chirality. (c) Correspondence between Fermi-arc endpoints and Weyl fermion nodes bolsters the case for Weyl fermions. (d) Illustration of the simplest Weyl semimetal state with two Weyl nodes with opposite (±1) chiral charges in the bulk. A corresponding surface Fermi arc is shown above. (Images and data by Su-Yang Xu and M. Zahid Hasan.)**