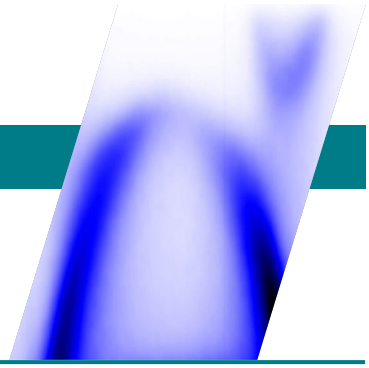
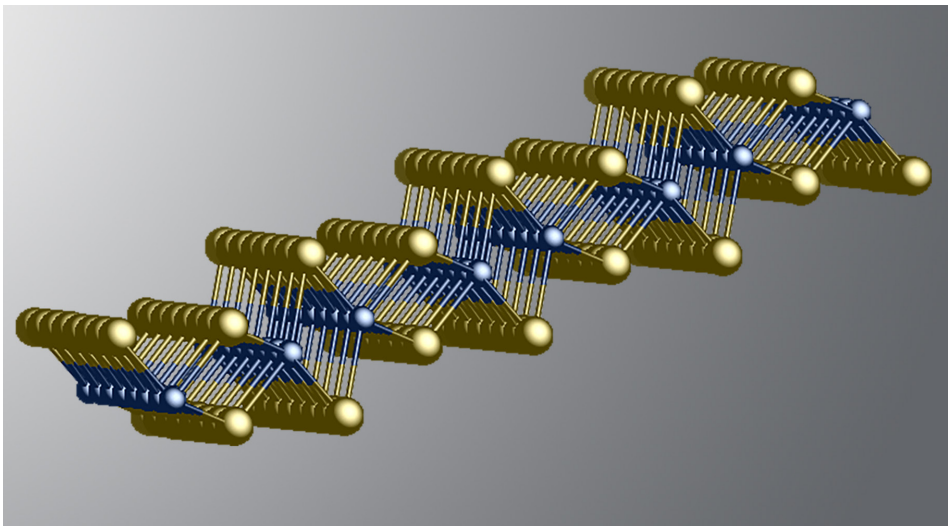


MATERIALS SCIENCES

Researchers Confirm New 2D Topological Insulator



The crystal structure of a 1T′-WTe_2 monolayer. (Credit: Berkeley Lab)

An international team of researchers fabricated an atomically thin layer of tungsten ditelluride (WTe_2) and measured the exotic and durable properties that make it a promising candidate for spintronic applications. Angle-resolved photoemission spectroscopy (ARPES) at the ALS, combined with scanning tunneling microscopy (STM) experiments and first-principles calculations, have established that a particularly stable form of WTe_2, the 1T′ structural phase (or "polytype"), is a two-dimensional topological insulator, confirming recent predictions. The findings should provide new opportunities for fundamental studies of topological phenomena and for next-generation spintronic applications.

The material under study, 1T′- WTe_2, bridges two flourishing fields of research: that of so-called 2D materials, which include monolayer materials such as graphene that behave in different ways than their thicker forms, and topological materials, in which electrons can zip around in predictable ways with next to no resistance and regardless of the usual (nonmagnetic) defects that would ordinarily impede their movement. The material is called a topological insulator because its interior does not conduct electricity; its electrical conductivity is restricted to its edges. There, the direction in which the electrons flow is completely linked to the direction of their spins, a useful quality for spintronic devices. Such devices could conceivably carry data more fluidly, with lower power demands and less heat buildup than is typical in present-day electronic devices.

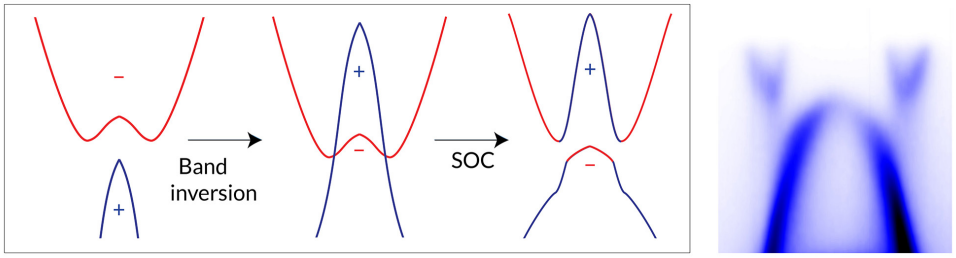
Three-atom-thick crystalline samples of the material were grown on a bilayer graphene substrate in a highly purified, vacuum-sealed compartment at the ALS, using molecular-beam epitaxy. The high-purity samples were then studied at Beamline 10.0.1 using ARPES, which provides a powerful probe of a material's electronic properties. In the resulting data, the researchers immediately recognized two characteristic signatures of a 2D topological insulator: an inversion of the conduction and valence bands (caused by the 1T′ structural distortion) and a band-gap opening (caused by spin-orbit coupling).

On the Edge of Discovery

Scientists at the Massachusetts Institute of Technology [Qian et al., *Science* **346**, 1344 (2014)] predicted in 2014 that a family of two-dimensional materials known as transition-metal dichalcogenides (TMDCs) would prove to be topological insulators—electrically insulating in the middle but conducting on the edges. The prediction sparked intense efforts to fabricate the material and demonstrate its characteristics in the lab. Toward that end, the work reported here began in 2015, led by Z.-X. Shen (SLAC and Stanford) and S.-K. Mo (ALS). It involved more than two dozen researchers in a variety of disciplines, from five countries across three continents. The work also benefited from the use of high-performance computing at Berkeley Lab's National Energy Research Scientific Computing Center (NERSC). At the same time, another group, from the University of Washington [Fei et al., *Nat. Phys.* **13**, 677 (2017)], published similar results using completely different, complementary methods. The rapid progress being made in this area owes much to advancements in theory, computation, fabrication, and characterization. With continued interplay between these modalities, the researchers expect TMDCs to be the material of choice for an expanded effort to understand and utilize topological materials, enabling the field to develop even faster.

Because the conducting part of the material, at its outermost edge, was only a few nanometers thick—thousands of times smaller than the x-ray beam's focus—additional experiments using scanning tunneling microscopy (STM) were performed to measure the local density of electron states there. Comparison of the data obtained from the edges vs from the bulk showed a much higher conductance at the edges, as expected for a 2D topological insulator.

Two-dimensional materials have unique electronic properties that are considered key to adapting them for various applications, and there is a very active worldwide research and development effort focused on tailoring these materials for specific uses by selectively stacking different types. Researchers are trying to sandwich them on top of each other to tweak the material as they wish—like Lego blocks. Now, with experimental proof of this material's properties, the goal is to stack it with other materials to see how these properties change.



Left: Schematic diagrams showing the evolution of band structure from a topologically trivial phase, to a nontrivial phase with band inversion, to the development of a band gap due to spin-orbit coupling (SOC); red = conduction band, blue = valence band. Right: The ARPES data for WTe_2 along the Γ–Y direction exhibits both band inversion and a band gap.

A typical problem in creating such designer materials from atomically thin layers is that materials often have nanoscale defects that can be difficult to eliminate and that can affect their performance. But because 1T′-WTe_2 is a topological insulator, its electronic properties are by nature resilient. At the nanoscale it may not be a perfect crystal, but the beauty of topological materials is that even when you have less-than-perfect crystals, the edge states survive. The imperfections don't break the key properties.

Going forward, the researchers aim to develop larger samples of the material and to discover how to selectively tune and accentuate specific properties. Besides its topological properties, its "sister materials," which have similar properties and were also studied by the research team, are known to be light-sensitive and have useful properties for solar cells and for optoelectronics, which control light for use in electronic devices.

Publication about this research: S. Tang, C. Zhang, D. Wong, Z. Pedramrazi, H.-Z. Tsai, C. Jia, B. Moritz, M. Claassen, H. Ryu, S. Kahn, J. Jiang, H. Yan, M. Hashimoto, D. Lu, R.G. Moore, C.-C. Hwang, C. Hwang, Z. Hussain, Y. Chen, M.M. Ugeda, Z.Liu, X. Xie, T.P. Devereaux, M.F. Crommie, S.-K. Mo, and Z.-X. Shen, "Quantum spin Hall state in monolayer 1T′ -WTe_2," *Nat. Phys.* **13**, 683 (2017). doi:10.1038/nphys4174.

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