Visualizing the topology of electrons with '3D glasses'

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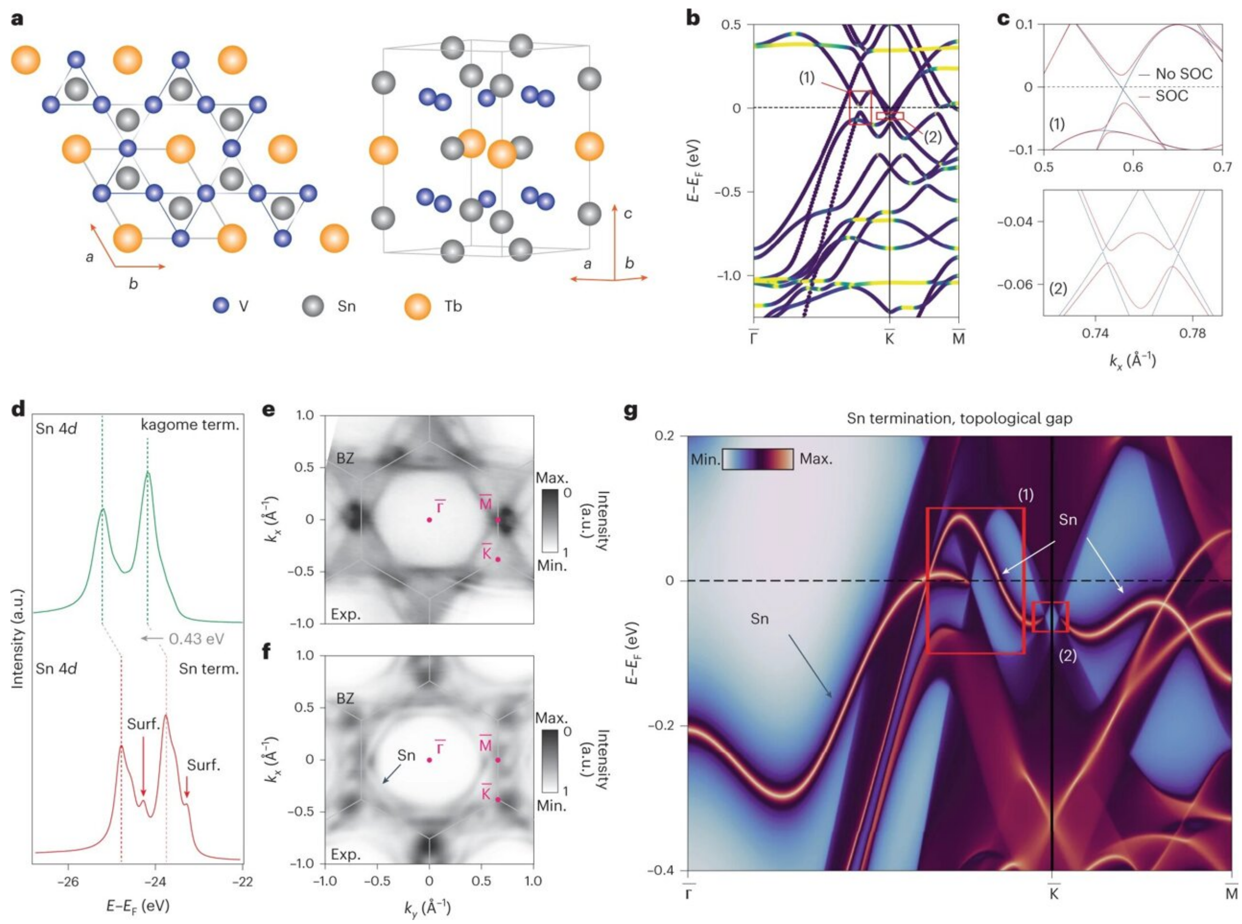

Crystal structure, bulk electronic properties and surface terminations of TbV_6Sn_6 kagome metal. **a**, Crystal structure of TbV_6Sn_6 showing top and side views of the unit cell. **b**, Bulk electronic structure along the Γ–K–M direction in the presence of SOC. The electronic states are colored by the band and momentum-resolved density of states, with yellow highlighting a large contribution. **c**, Enlargement of the red boxes (1) and (2) in **b**. Red and blue bands refer to calculations with and without SOC, respectively. **d**, Sn 4*d* core level spectroscopy for the kagome-terminated (term.) (green) and Sn-terminated (red) surface (surf.) of TbV_6Sn_6. **e**,**f**, ARPES Fermi surfaces for the kagome (**e**) and Sn (**f**) termination of TbV_6Sn_6, respectively. **g**, Spectral function of the (001) surface Green's function for the Sn termination in the absence of SOC. Boxes (1) and (2) refer to those in **b**. Credit: *Zenodo* (2023). DOI: 10.5281/zenodo.7787937

They are seen as a beacon of hope for energy-saving electronics and the high-tech of the future: topological quantum materials. One of their properties is the conduction of spin-polarized electrons on their surface—even though they are actually non-conductive inside. To put this into perspective: In spin-polarized electrons, the intrinsic angular momentum, i.e. the direction of rotation of the particles (spin), is not purely randomly aligned.

To distinguish topological materials from conventional ones, scientists used to study their surface currents. However, an electron's topology is closely linked to its quantum mechanical wave properties and its spin. This relationship has now been demonstrated directly by means of the photoelectric effect—a phenomenon in which electrons are released from a material, such as metal, with the aid of light.

Prof. Giorgio Sangiovanni, a founding member of ct.qmat in Würzburg and one of the theoretical physicists in the project, likened this discovery to using 3D glasses to visualize the topology of electrons. He explains, "Electrons and photons can be described quantum mechanically as both waves and particles. Therefore, electrons have a spin that we can measure thanks to the photoelectric effect."

To do this, the team used circularly polarized X-ray light—light particles possessing a torque. Sangiovanni elaborates, "When a photon meets an electron, the signal coming from the quantum material depends on whether the photon has a right- or a left-handed polarization."

"In other words, the orientation of the electron's spin determines the relative strength of the signal between left- and right-polarized beams. Therefore, this experiment can be thought of like polarized glasses in a 3D cinema, where differently oriented beams of light are also used. Our '3D glasses' make electrons' topology visible."

Headed by the Würzburg-Dresden Cluster of Excellence ct.qmat—Complexity and Topology in Quantum Matter—this ground-breaking experiment, along with its theoretical description, is the first successful attempt at characterizing quantum materials topologically. Sangiovanni points out the essential role of a particle accelerator in the experiment, stating, "We need the synchrotron particle accelerator to generate this special X-ray light and to create the '3D cinema' effect."

Quantum matter, particle accelerators and supercomputers

The journey to this monumental success spanned a period of three years for the researchers. Their starting point was the kagome metal TbV_6Sn_6, a quantum material. In this special class of materials, the atomic lattice has a mixture of triangular and honeycomb lattices in a structure reminiscent of a Japanese basket weave. Kagome metals play an important role in ct.qmat's materials research.

"Before our experimental colleagues could start the synchrotron experiment, we needed to simulate the results to make sure we were on the right track. In the first step, we devised theoretical models and ran calculations on a supercomputer," says Dr. Domenico di Sante, the project lead and a theoretical physicist, who is also an associate member of the Würzburg Collaborative Research Center (SFB) 1170 ToCoTronics.

The findings from the measurements lined up perfectly with the theoretical predictions, enabling the team to visualize and confirm the topology of the kagome metals.

The paper is published on the *Zenodo* preprint server.

More information: Domenico Di Sante et al, Flat band separation and robust spin-Berry curvature in bilayer kagome metals, *Zenodo* (2023). DOI: 10.5281/zenodo.7787937

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