Mapping the curvature where electrons reside in Kagome materials

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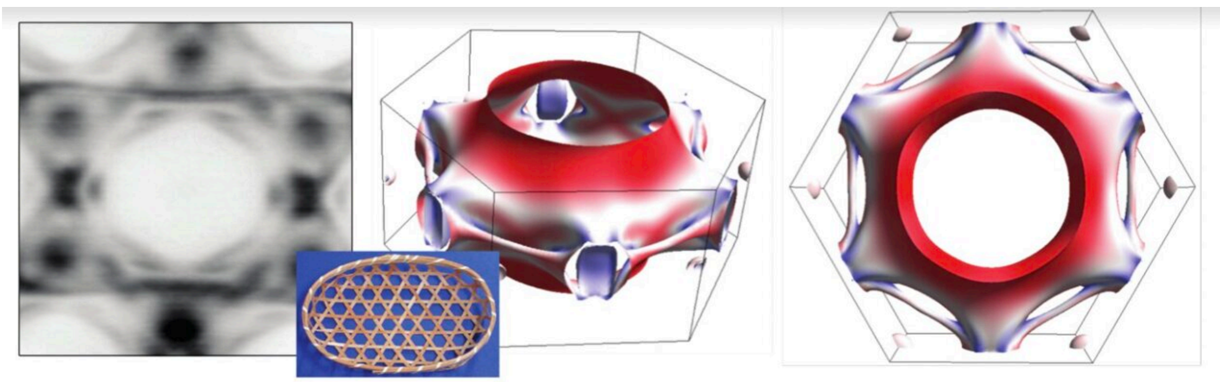

Three perspectives of the so-called Fermi surface of the studied material, i.e., the surface on which the electrons move. On the left, the experimental result, in the center and on the right the theoretical modeling. The red and blue colors represent a measure of the speed of the electrons. Both theory and experiment reflect the symmetries of crystal, present in the Japanese weave "kagome" used to make traditional baskets. Credit: Di Sante et al

Kagome metals are a class of quantum materials with interesting properties that are characterized by a unique lattice structure resembling Japanese woven bamboo patterns of the same name (i.e., Kagome). Over the past decade, physicists have been using these materials to study various electronic phenomena resulting from their unique structure.

Researchers at University of Bologna, University of Venice, CNR-IOM of Trieste, University of Würzburg, and other institutes in Europe and the U.S. recently carried out a study investigating the spin and electronic structure of XV_6Sn_6, materials, a family of Kagome metals that is partly composed of a rare-earth element. Their paper, published in *Nature Physics*, maps the behavior of electrons residing in a curved space within the materials, which is known as spin Berry curvature.

"Kagome metals belong to a class of new quantum materials that is revolutionizing the way material scientists look at complex collective phenomena, such as magnetism and superconductivity," Domenico Di Sante, one of the researchers who carried out the study, told Phys.org. "We have been working on Kagome metals for several years, and this paper came out as a natural continuation of our previous works. The primary objective was to detect the curvature of the space where some of the electrons in Kagome metals live."

Di Sante and his colleagues set out to explore the spin Berry curvature in the XV_6Sn_6 Kagome family using both theoretical and experimental methods. They first simulated the materials using advanced computing software and then used a technique called angle-resolved photoemission spectroscopy to examine samples of the Kagome metal ScV_6Sn_6.

"From the theoretical viewpoint we used modern and very powerful supercomputers to model, via sophisticated software, the behavior of electrons inside the Kagome metals," Di Sante said. "From the experimental side, we needed to use the light that can be generated only at large-scale facilities such as synchrotrons to detect the energy and velocity of the electrons, simultaneously to their spin."

The simulations and experiments conducted by the researchers led to some interesting observations. Specifically, they gathered evidence of a finite spin Berry curvature at the center of the Brillouin zone, At this curvature, the materials' nearly flat band was found to detach from the so-called Dirac band, due to a physical phenomenon known as spin-orbit coupling. When they examined a sample of ScV_6Sn_6, the team found that in this material the spin Berry curvature was robust against the onset of an ordered phase driven by changes in temperature.

"The most notable contribution of our work is the application of a well-defined protocol, i.e., the use of light, circular dichroism and spin resolution, to map out the curved space where the electrons live," Di Sante said. "In a similar way the space-time of our universe is curved by matter, stars, galaxies, black holes etc, the space where the electrons move can be curved. Our work detected one of these curvatures in Kagome metals."

The recent work by this team of researchers gathered new valuable insight about the electronic structure and spectroscopic fingerprint of Kagome metals in the XV_6Sn_6 family. In the future, their observations could pave the way for new studies assessing the unique qualities of these materials and their possible technological applications.

"In our next works, we plan to continue investigating this class of materials," Di Sante added. "There are other families of Kagome metals that promise to enrich our understanding of collective phenomena and their link to the field of topology (curved spaces are intimately link to the concept of topology)."

More information: Domenico Di Sante et al, Flat band separation and robust spin Berry curvature in bilayer kagome metals, *Nature Physics* (2023). DOI: 10.1038/s41567-023-02053-z

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