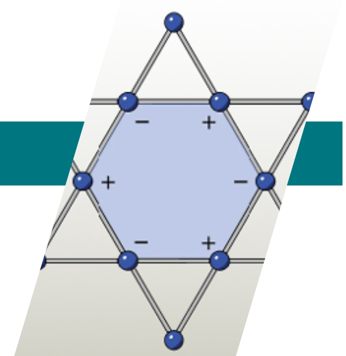
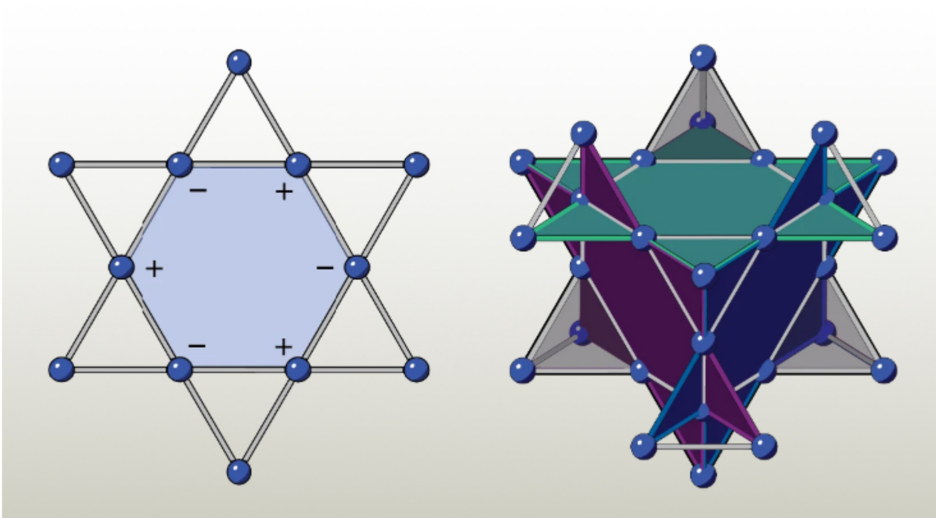
ADVANCED LIGHT SOURCE

MATERIALS SCIENCES

Flat Bands Signal Electrons Trapped in 3D





Inspired by 2D "kagome" patterns (left) that are known to trap electrons in the hexagonal areas (blue) defined by corner-sharing triangles, the "pyrochlore" structure (right) has four hexagonal planes (teal, purple, blue, and gray) that trap electrons in localized states in 3D, leading to greater electron–electron interactions and exotic properties such as superconductivity. (Credit: Massachusetts Institute of Technology)

Scientific Achievement

Using the Advanced Light Source (ALS), researchers found flat electronic band structures—known hallmarks of electrons trapped in two dimensions—but in a material that extends this phenomenon to three dimensions.

Significance and Impact

The work opens up a material framework for exploring superconductivity and other exotic states in three dimensions for advanced electronic applications.

A new dimension in exotic physics

When a material's electrons are trapped together, they can settle into the same energy state and start to behave as one. In this collective state, the electron energies remain constant no matter what their momentum values are. In angle-resolved photoemission spectroscopy (ARPES) experiments, which map electron energy versus momentum, this state is signaled by a flat band in the data. Scientists predict that when electrons are in this state, they can start to feel the quantum effects of other electrons and act in coordinated, quantum ways. Then, exotic behavior such as superconductivity and unique forms of magnetism may emerge.

In this work, a team led by researchers from the Massachusetts Institute of Technology (MIT) have found a three-dimensional material that exhibits this distinctive flat-band signature in ARPES data, previously observed only for two-dimensional systems. With some chemical manipulation, the researchers also showed that they could transform the crystal into a superconductor—a material that conducts electricity with zero resistance.

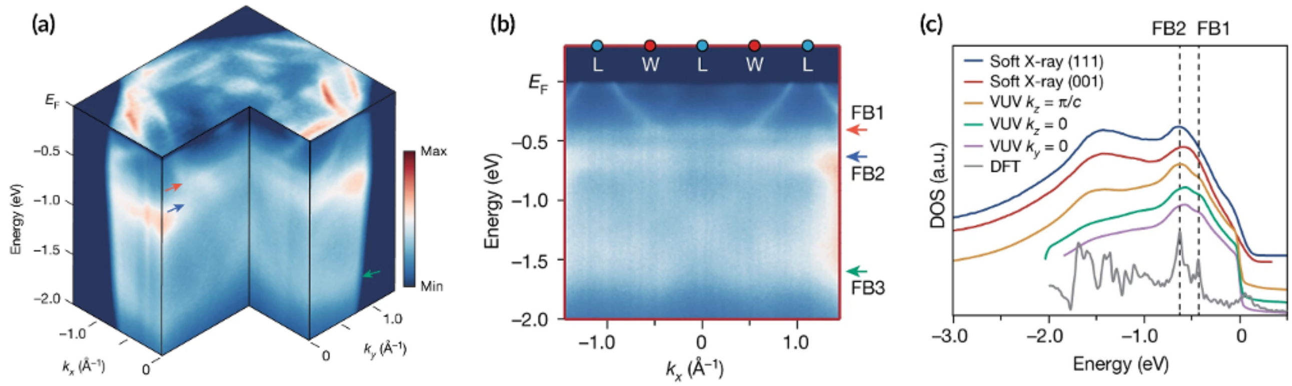
Setting a 3D trap

In work previously done at the ALS, the team observed that a two-dimensional lattice of interconnected, corner-sharing triangles (resembling Japanese "kagome" basket-weaving patterns) could confine electrons to the hexagonal space circumscribed by the triangles. But they and others also found that the electrons could escape up and out through the third dimension.

The team wondered: Could a three-dimensional configuration of similar lattices work to box in the electrons? In databases of material structures, they came across an atomic configuration associated with minerals known as pyrochlores. This structure forms a repeating pattern of cubes, with the face of each cube resembling a kagome-like lattice. The team found that, in theory, this geometry could effectively trap electrons within each cube.

Flat bands materialize

To test this hypothesis, the researchers synthesized a pyrochlore metal, $CaNi_2$. Because the surface of this material is highly corrugated, photoemission studies of its electronic behavior require an ultrafocused beam of light capable of targeting specific locations across the uneven surface.



(a) Three-dimensional view of the VUV ARPES data. (b) A vertical slice through the data in (a) highlighting the three flat bands (FB1, FB2, and FB3). (c) Comparison of the momentum-integrated ARPES spectra obtained using VUV and soft x-ray ARPES measurements. The peaks in the experimental spectra are consistent, supporting the bulk origin of the flat bands. The grey curve shows the density of states obtained from density functional theory (DFT) calculations.

The sample was probed using vacuum ultraviolet (VUV) ARPES at ALS Beamline 7.0.2 (MAESTRO). Additional VUV and soft x-ray ARPES work was done at the National Synchrotron Light Source II (NSLS-II) and the Advanced Photon Source (APS), respectively. With the beamlines' small spot sizes and ability to tune the photon energy, the researchers were able to directly observe extremely narrow bands in all three dimensions.

The data revealed three flat bands, at –0.41 ± 0.03 eV, –0.58 ± 0.03 eV, and –1.58 ± 0.05 eV. Theoretical models and further studies of electronic behavior using quantum oscillation measurements helped substantiate that the observed spectra are of bulk origin.

A glimpse at future possibilities

Finally, the researchers were able to chemically tune one of the flat bands by replacing the nickel in $CaNi_2$ with a mixture of rhodium and ruthenium. This coincided with the appearance of superconductivity at a temperature of 6.2 K. From this point on, the researchers say, the challenge is to optimize flat-band materials to sustain superconductivity at higher temperatures. Such materials might someday enable ultra-efficient power lines, supercomputing quantum bits, and faster, smarter electronic devices.

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