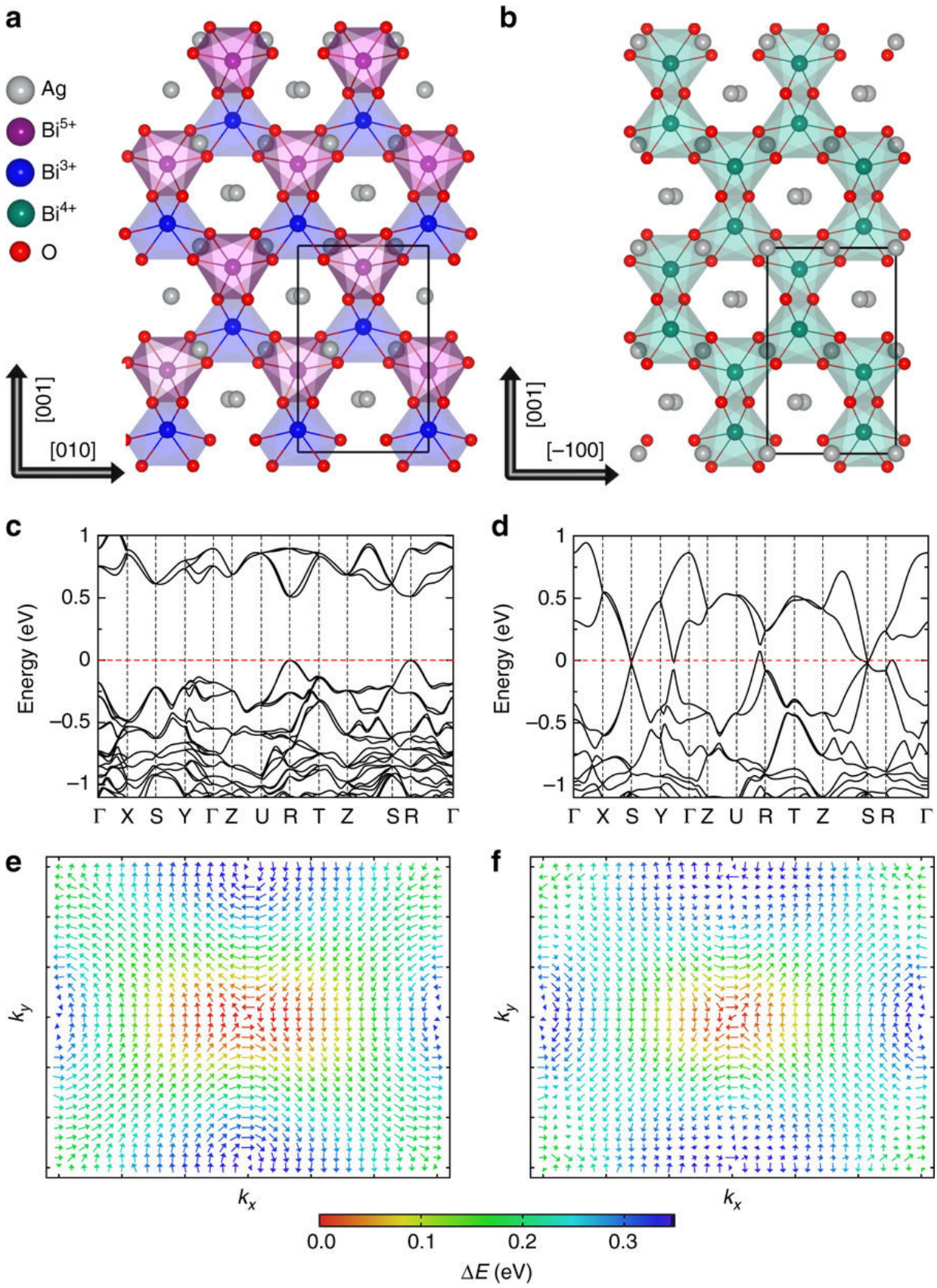
Controlling quantum interactions in a single material

February 5 2018


a
Ag
Bi5+
Bi3+
Bi4+
O
[001]
[010]
b
[001]
[−100]
c
Energy (eV)
1
0.5
0
−0.5
−1
Γ X S Y Γ Z U R T Z SR Γ
d
Energy (eV)
1
0.5
0
−0.5
−1
Γ X S Y Γ Z U R T Z SR Γ
e
ky
kx
f
ky
kx
0.0
0.1
0.2
0.3
ΔE (eV)

Structural and electronic properties of Ag2BiO3. Crystal structure of a the ferroelectric Pnn2 and b the hypothetical paraelectric Pnna phase. Red, gray, green, blue, and purple spheres are O2−, Ag+, Bi4+, Bi3+, and Bi5+ ions, respectively. c and d are the band structures of the Pnn2 and Pnna phases, respectively. The Fermi level is shifted to 0 eV. High symmetry points in the first Brillouin zone are defined in Supplementary Figure 1. e and f are the spin textures of the inner and outer branches of conduction bands at the R point in the polar Pnn2 phase. The color code indicates the energy level with respect to the bottom of conduction band. Credit: *Nature Communications* (2018). DOI: 10.1038/s41467-017-02814-4

The search and manipulation of novel properties emerging from the quantum nature of matter could lead to next-generation electronics and quantum computers. But finding or designing materials that can host such quantum interactions is a difficult task.

"Harmonizing multiple quantum mechanical properties, which often do not coexist together, and trying to do it by design is a highly complex challenge," said Northwestern University's James Rondinelli.

But Rondinelli and an international team of theoretical and computational researchers have done just that. Not only have they demonstrated that multiple quantum interactions can coexist in a single material, the team also discovered how an electric field can be used to control these interactions to tune the material's properties.

This breakthrough could enable ultrafast, low-power electronics and quantum computers that operate incredibly faster than current models in the areas of data acquisition, processing, and exchange.

Supported by the US Army Research Office, National Science

Foundation of China, German Research Foundation, and China's National Science Fund for Distinguished Young Scholars, the research was published online today in the journal *Nature Communications*. James Rondinelli, the Morris E. Fine Junior Professor in Materials and Manufacturing in Northwestern's McCormick School of Engineering, and Cesare Franchini, professor of quantum materials modeling at the University of Vienna, are the paper's co-corresponding authors. Jiangang He, a postdoctoral fellow at Northwestern, and Franchini served as the paper's co-first authors.

Quantum mechanical interactions govern the capability of and speed with which electrons can move through a material. This determines whether a material is a conductor or insulator. It also controls whether or not the material exhibits ferroelectricity, or shows an electrical polarization.

"The possibility of accessing multiple order phases, which rely on different quantum-mechanical interactions in the same material, is a challenging fundamental issue and imperative for delivering on the promises that quantum information sciences can offer," Franchini said.

Using computational simulations performed at the Vienna Scientific Cluster, the team discovered coexisting quantum-mechanical interactions in the compound silver-bismuth-oxide. Bismuth, a post-transition metal, enables the spin of the electron to interact with its own motion—a feature that has no analogy in classical physics. It also does not exhibit inversion symmetry, suggesting that ferroelectricity should exist when the material is an electrical insulator. By applying an electric field to the material, researchers were able to control whether the electron spins were coupled in pairs (exhibiting Weyl-fermions) or separated (exhibiting Rashba-splitting) as well as whether the system is electrically conductive or not.

"This is the first real case of a topological quantum transition from a ferroelectric insulator to a non-ferroelectric semi-metal," Franchini said. "This is like awakening a different kind of quantum interactions that are quietly sleeping in the same house without knowing each other."

More information: Jiangang He et al, Tunable metal-insulator transition, Rashba effect and Weyl Fermions in a relativistic charge-ordered ferroelectric oxide, *Nature Communications* (2018). DOI: 10.1038/s41467-017-02814-4

Provided by Northwestern University