Researchers discover new flat electronic bands, paving way for advanced quantum materials

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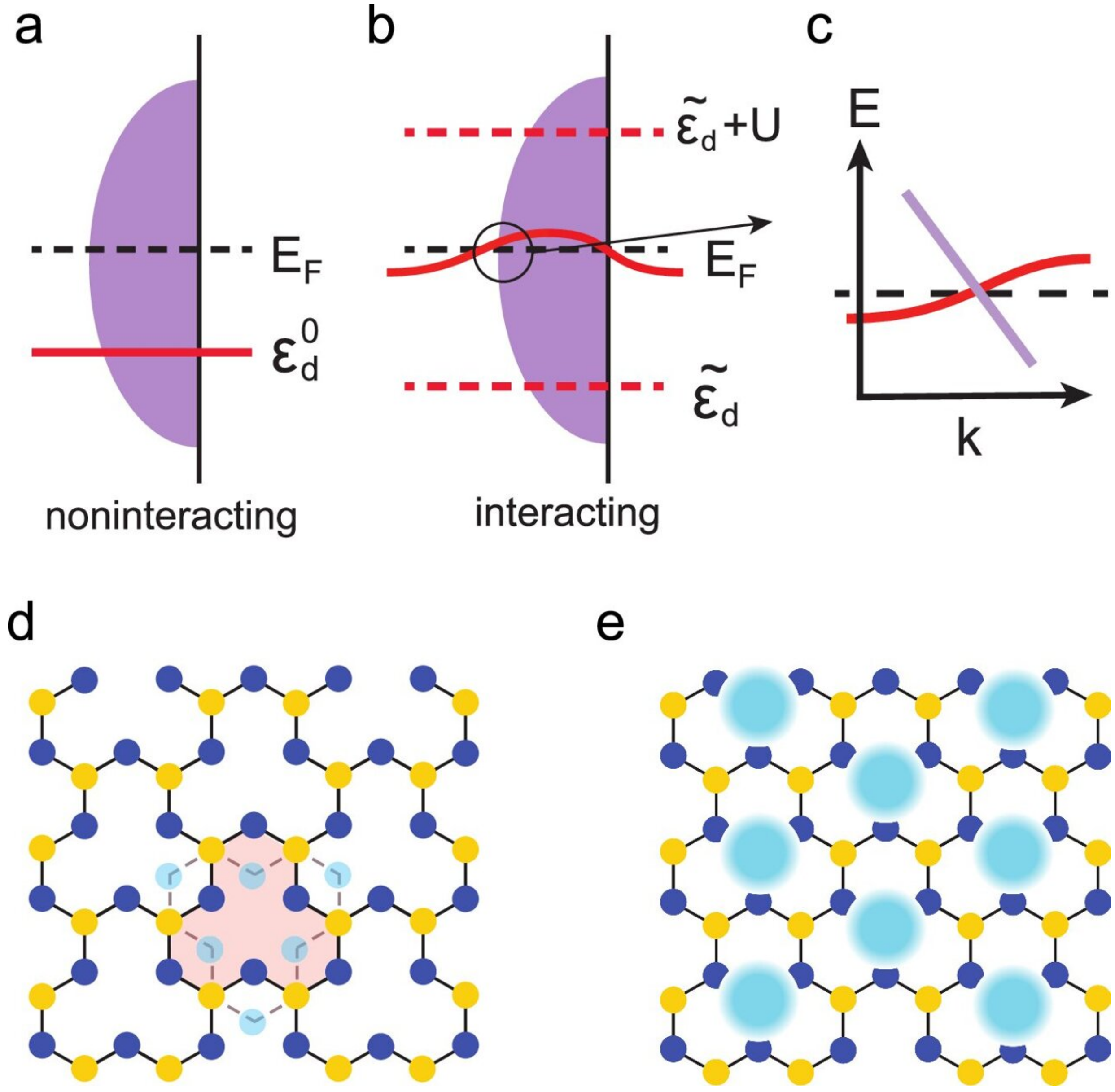

Illustration of the bare and emergent flat bands and lattice geometry. a In the noninteracting case, a flat band (red solid line) appears far away from the Fermi energy. b In the presence of orbital-selective correlations, an interaction-driven flat band emerges at the Fermi energy (red solid line), while leaving incoherent excitations far away from the Fermi energy (red dashed lines). c The emergent flat band crosses a dispersive band, leading to a topological Kondo semimetal with symmetry-protected Dirac/Weyl nodes that are pinned close to the Fermi energy, within an effective Kondo energy scale. d Geometry of the clover lattice with 5 sublattices per unit cell. The lattice does not have inversion symmetry. This can be seen from the mismatch between the (dark) blue sublattices and their inversion counterparts (dots in light blue). e The Wannier orbitals are near the geometric centers (shaded blue circles) of the unit cells, which form a triangular lattice. Credit: *Nature Communications* (2024). DOI: 10.1038/s41467-024-49306-w

In a study published in *Nature Communications*, a team of scientists led by Rice University's Qimiao Si predicts the existence of flat electronic bands at the Fermi level, a finding that could enable new forms of quantum computing and electronic devices.

Quantum materials are governed by the rules of quantum mechanics, where electrons occupy unique energy states. These states form a ladder with the highest rung called the Fermi energy.

Electrons, being charged, repel each other and move in correlated ways. Si's team found that electron interactions can create new flat bands at the Fermi level, enhancing their importance.

"Most flat bands are located far from the Fermi energy, which limits their impact on the material's properties," said Si, the Harry C. and Olga

K. Wiess Professor of Physics and Astronomy at Rice.

Typically, a particle's energy changes with its momentum. But in quantum mechanics, electrons can exhibit quantum interference, where their energy remains flat even when their momentum changes. These are known as flat bands.

"Flat electronic bands can enhance electron interactions, potentially creating new quantum phases and unusual low-energy behaviors," Si said.

These bands are especially sought after in transition metal ions called d-electron materials with specific crystal lattices, where they often show unique properties, Si said.

The team's findings suggest new ways to design these, which could inspire new applications for these materials in quantum bits, qubits and spintronics. Their research shows that electron interactions can link immobile and mobile electron states.

Using a theoretical model, the researchers demonstrated that these interactions can create a new type of Kondo effect, where immobile particles gain mobility by interacting with mobile electrons at the Fermi energy. The Kondo effect describes the scattering of conduction electrons in a metal due to magnetic impurities, resulting in a characteristic change in electrical resistivity with temperature.

"Quantum interference can enable the Kondo effect, allowing us to make significant progress," said Lei Chen, a Ph.D. student at Rice.

A key attribute of the flat bands is their topology, Chen said. "The flat bands pinned to the Fermi energy provide a means to realize new quantum states of matter," he said.

The team's research reveals that this includes anyons and Weyl fermions, or massless quasiparticles and fermions that carry an electric charge. The researchers found that anyons are promising agents for qubits, and materials that host Weyl fermions may find applications in spin-based electronics.

The study also highlights the potential for these materials to be very responsive to external signals and capable of advanced quantum control. The results indicate that the flat bands could lead to strongly correlated topological semimetals at relatively low temperatures, potentially operating at high temperatures or even room temperature.

"Our work provides the theoretical foundation for utilizing flat bands in strongly interacting settings to design and control novel quantum materials that operate beyond the realm of low temperatures," Si said.

Contributors to this research include Fang Xie and Shouvik Sur, Rice postdoctoral associates of physics and astronomy; Haoyu Hu, Rice alumnus and postdoctoral fellow at Donostia International Physics Center; Silke Paschen, physicist at the Vienna University of Technology; and Jennifer Cano, theoretical physicist at Stony Brook University and the Flatiron Institute.

More information: Lei Chen et al, Emergent flat band and topological Kondo semimetal driven by orbital-selective correlations, *Nature Communications* (2024). DOI: 10.1038/s41467-024-49306-w

Provided by Rice University

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