Itinerant magnetism and superconductivity in exotic 2D metals for next-generation quantum devices

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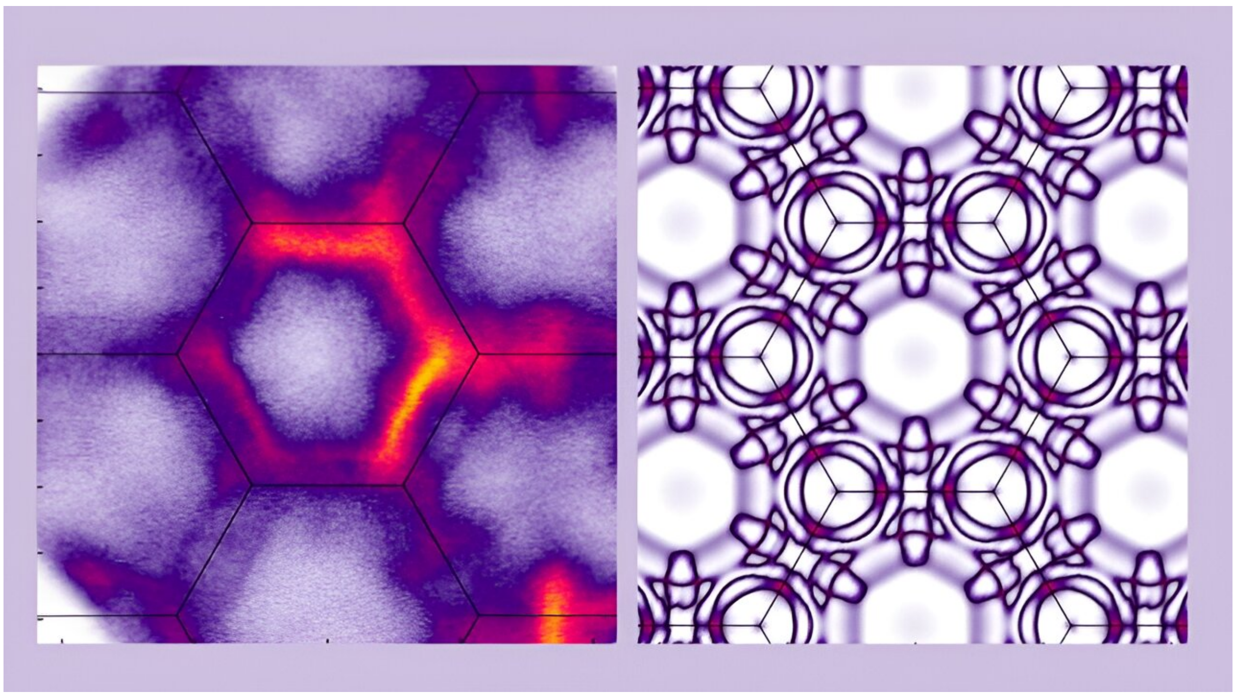

Electronic structure measurements and calculations of $NiTa_4Se_8$. Credit: Berkeley Lab

The Quantum Systems Accelerator (QSA) pioneers studies to build and co-design the next generation of programmable quantum devices. An interdisciplinary team of scientists from QSA institutions, Lawrence

Berkeley National Laboratory (Berkeley Lab), and the University of California, Berkeley (UC Berkeley), in collaboration with Los Alamos National Laboratory, conducted a series of experiments with a new type of layered 2D metal, finding connections in electronic behavior that might potentially be useful for fabricating complex superconducting quantum processors.

The research with this new transition metal dichalcogenide (TMD) leverages teams of experts at Berkeley Lab collaborating and co-designing across different fields while leveraging state-of-the-art national capabilities and instrumentation at the Advanced Light Source and Molecular Foundry. *Physical Review B* published the experimental results in December 2022.

Novel experiments for a deeper understanding of the physics of new materials

Searching for new superconducting 2D materials can provide clues to many of the fabrication and materials challenges of superconducting quantum processors currently using conventional materials such as aluminum, niobium, and silicon.

TMDs are exotic metals that can naturally be fabricated into very thin layers with a well-defined crystalline structure ideally suited for experimentation and devices. They display unique physical properties from the interactions of their electrons.

The electrons can be localized to a few atoms interacting more strongly with each other. The densely packed, closely interacting electrons can trigger unique properties and behaviors such as superconductivity and itinerant magnetism. Superconductivity enables the movement of an electrical charge through the metal with little to no resistance. Itinerant magnetism occurs when electrons transfer magnetism from one atom to another instead of being localized to a fixed position.

An important finding in the scientific literature is that materials are generally superconductors or magnets, but not both. However, the itinerant magnetism phase is close to the superconductivity transition. Hence, detecting strong magnetic properties in the crystalline structure of a TMD is a great starting point for searching for new superconductors. But, the degree to which the interplay of itinerant magnetism and superconductivity are found in TMDs has not been well understood.

$NiTa_4Se_8$ is an emerging class of intercalated TMD with strongly correlated electrons that move in two-dimensional planes with a ferromagnetic (nickel) layer, making the interaction or correlation between electrons stronger. QSA researchers involved in the series of experiments characterized the electronic conduction properties—transport properties—in $NiTa_4Se_8$, observing both itinerant magnetism and superconductivity.

"I find it very inspiring that physical laws are often related to an understanding of symmetries, so when I'm studying new materials that have unique internal symmetries, be the configuration of different atoms or what their local or global environment is, I know it will result in a different set of properties for the system," said James Analytis, associate professor at UC Berkeley and faculty scientist at Berkeley Lab, is the paper's experimental lead.

To study the properties of superconductivity and itinerant magnetism, the researchers needed to understand the internal symmetries of the material. Analytis and the team synthesized the different symmetry configurations in $NiTa_4Se_8$, manipulating the system of atoms and electrons in the layered crystalline metal through various chemical processing and techniques.

The series of experiments allowed researchers to study how electrons behaved in $NiTa_4Se_8$ by stacking, manipulating, and controlling them in the laboratory.

Advanced tools and expertise at DOE National Facilities at Berkeley Lab

For the Materials Sciences' Division and Molecular Foundry's Sinéad Griffin, one of the paper's co-authors and QSA materials topical group research lead, discovering new superconductors is a top priority for the next-generation superconducting quantum technologies. Griffin develops theoretical models and calculations that predict material properties to guide fabrication and characterization at the lab.

"I'm motivated to find a new type of physics or system that no one has seen before, so the opportunity to have this playground of facilities and instrumentation at Berkeley Lab while being close to the team doing the experimentations and measurements is key. We're not limited by what's available. We're more limited by our imagination," said Griffin.

The team leveraged Berkeley Lab's cutting-edge photoelectron spectroscopy capabilities at the ALS, which uses photons to interact with electrons for more rapid characterization of 2D materials and surfaces, including Angle-Resolved Photoemission Spectroscopy (ARPES) and Energy-dispersive X-ray spectroscopy (EDS or EDX), as well as powder X-ray diffraction to simulate, characterize, and study the complex crystalline structure of $NiTa_4Se_8$ at the finest of scales.

Eli Rotenberg, a staff scientist at the ALS and QSA researcher, is fascinated by quantum materials with exotic physical properties from the interactions of their electrons. An expert in photoelectron spectroscopy, Rotenberg took detailed measurements of the electrons' behavior and the so-called Fermi surface, an important energy level in condensed matter physics for superconductivity with exquisite precision.

"Crystals are like a glass of water, filled up to a point and empty above where electrons near the surface participate in electrical conduction. The interesting physics of these crystalline materials comes at the interface between occupied and unoccupied states. Particles can be excited from the occupied to the unoccupied side to form moving waves that transmit energy information," explained Rotenberg.

Co-designing accelerates fundamental discovery

The complexity of the novel materials being studied to build better quantum devices and the variety of measurements to understand them requires state-of-the-art instrumentation and tools where each technique is specific to a system. Materials properties often change, or defects emerge as they get built into quantum devices,

"You're almost asking the reverse question when you ask how do I find this new type of phenomenon that no one has found or this result in that system or material. Using theory, I can try designing a material from the fundamental key ingredients," said Griffin.

$NiTa_4Se_8$ is likely not unique among the magnetic TMDs. Therefore, the team concluded that searching for correlated itinerant magnetism and unconventional superconductivity in 2D materials can refine the understanding of the materials that could potentially be used to fabricate increasingly complex quantum processors.

However, researchers need to continue to understand better the fundamental levels of these types of 2D materials. QSA continues to explore the solutions to many fabrication challenges that will help bridge today's imperfect hardware systems with those capable of impactful science.

"Having a single team with a singular vision, like in QSA, that has all the tools available accelerates the process from fundamental science to technologies. You often have to explore which technique or synthesis capabilities are better suited for different materials," concluded Analytis.

More information: Nikola Maksimovic et al, Strongly correlated itinerant magnetism near superconductivity in NiTa4Se8, *Physical Review B* (2022). DOI: 10.1103/PhysRevB.106.224429

Provided by Lawrence Berkeley National Laboratory

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