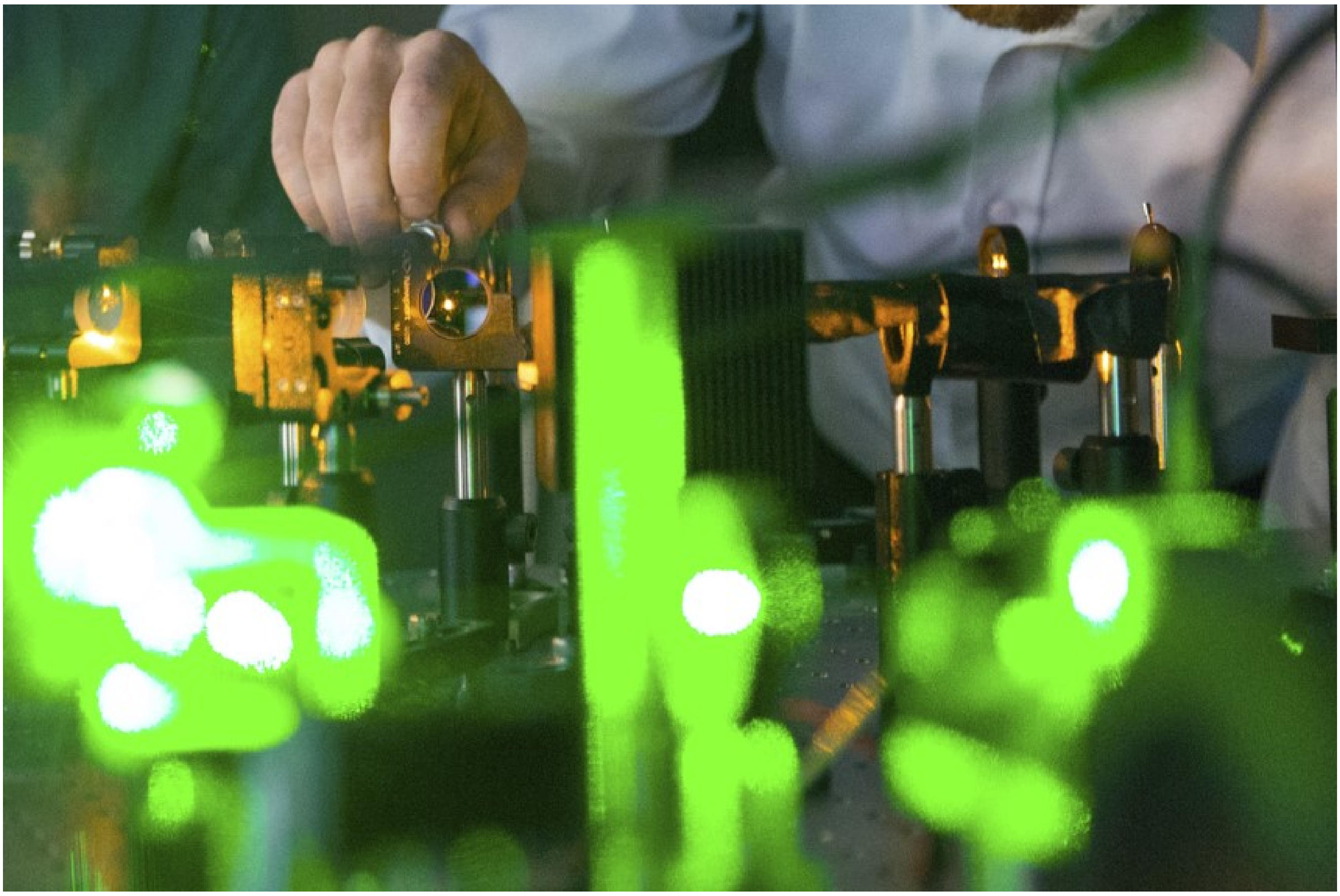
SCIENCE & TECHNOLOGY

Uncovering unexpected properties in a complex quantum material

Using a novel technique developed at Penn, researchers gained new insights into the properties of a proposed excitonic insulator known as Ta2NiSe5, with implications for future quantum devices.



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A new study describes previously unexpected properties in a complex quantum material known as Ta_2NiSe_5. Using a novel technique developed at Penn, these findings have implications for developing future quantum devices and applications. This research, published in *Science Advances* (https://www.science.org/doi/10.1126/sciadv.abl9020), was conducted by graduate student Harshvardhan Jog (https://agarwal.seas.upenn.edu/people/phds) and led by professor Ritesh Agarwal (https://directory.seas.upenn.edu/ritesh-agarwal/) in collaboration with Penn's Eugene Mele (https://live-sas-physics.pantheon.sas.upenn.edu/people/standing-faculty/eugene-mele) and Luminita Harnagea (file:///Users/riteshagarwal/Library/Containers/com.apple.mail/Data/Library/Mail%20Downloads/FDE7A52E-61AE-4BA2-9742-6A661BFD07E2/Luminita%20Harnagea) from the Indian Institute of Science Education and Research (https://www.iiserpune.ac.in/).

While the field of quantum information science (https://en.wikipedia.org/wiki/Quantum_information_science) has experienced progress in recent years, the widespread use of quantum computers is still limited. One challenge is the ability to only use a small number of "qubits," the unit that performs calculations in a quantum computer, because current platforms are not designed to allow multiple qubits to "talk" to one another. In order to address this challenge, materials need to be efficient at quantum entanglement (https://en.wikipedia.org/wiki/Quantum_entanglement), which occurs when the states of qubits remain linked no matter their distance from one another, as well as coherence, or when a system can maintain this entanglement.

In this study, Jog looked at Ta_2NiSe_5, a material system that has strong electronic correlation, making it attractive for quantum devices. Strong electronic correlation means that the material's atomic structure is linked to its electronic properties and the strong interaction that occurs between electrons.

To study Ta_2NiSe_5, Jog used a modification of a technique developed in the Agarwal lab known as the circular photogalvanic effect, where light is engineered to carry an electric field and is able to probe different material properties. Developed and iterated in the past several years, this technique has revealed insights about materials such as silicon (https://penntoday.upenn.edu/news/penn-researchers-discover-new-chiral-property-silicon-photonic-applications) and Weyl semimetals (https://penntoday.upenn.edu/news/unique-electrical-properties-quantum-materials-can-be-controlled-using-light) in ways that are not possible with conventional physics and materials science experiments.

But the challenge in this study, says Agarwal, is that this method has only been applied in materials without inversion symmetry, whereas Ta_2NiSe_5 does haveinversion symmetry, Jog "wanted to see if this technique can be used to study materials which have inversion symmetry which, from a conventional sense, should not be producing this response," says Agarwal.

After connecting with Harnagea to obtain high-quality samples of Ta_2NiSe_5, Jog and Agarwal used a modified version of the circular photogalvanic effect and were surprised to see that there was a signal being produced. After conducting additional studies to ensure that this was not an error or an experimental artifact, they worked with Mele to develop a theory that could help explain these unexpected results.

Mele says that the challenge with developing a theory was that what was hypothesized about the symmetry of Ta_2NiSe_5 did not align with the experimental results. Then, after finding a previous theory paper that suggested that the symmetry was lower than what was hypothesized, they were able to develop an explanation for these data. "We realized that, if there was a low temperature phase where the system would spontaneously shear, that would do it, suggesting that this material was deforming to this other structure," says Mele.

By combining their expertise from both experiment and theory, an essential component of the success of this project, the researchers found that this material had broken symmetry, a finding that has significant implications on using this and other materials in future devices. This is because symmetry plays a fundamental role in classifying phases of matter and, ultimately, in understanding what their downstream properties will be.

These results also provide a platform for finding and describing similar properties in other types of materials. "Now, we have a tool that can probe very subtle symmetry breaking in crystalline materials. To understand any complex material, you have to think about symmetries because it has huge implications," says Agarwal.

While there remains a "long journey" before Ta_2NiSe_5 can be incorporated into quantum devices, the researchers are already making progress on evaluating this phenomenon further. In the laboratory, Jog and Agarwal are interested in studying additional energy levels within Ta_2NiSe_5, looking for potential topological properties and using the circular photogalvanic method to study other correlated systems to see if they might also have similar properties. On the theory side, Mele is studying how prevalent this phenomena might be in other material systems and is developing suggestions for other materials for experimentalists to study in the future.

"What we're seeing here is a response that shouldn't occur but does under these circumstances," says Mele. "Expanding the space of structures that you have, where you can turn on these effects that are nominally forbidden, is really important. It's not the first time that's ever happened in spectroscopy, but, whenever it does occur, it's an interesting thing."

Along with presenting a new tool for studying complex crystals to the research community, this work also provides important insights into the types of materials that can provide two key features, entanglement and macroscopic coherence that are crucial for future quantum applications that range from medical diagnostics, low-power electronics, and sensors.

"The long-term idea, and one of the biggest goals of condensed matter physics, is to be able to understand these highly entangled states of matter because these materials themselves can do a lot of complex simulation," says Agarwal. "It could be that, if we can understand these types of systems, they can become natural platforms to do large-scale quantum simulation."

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CREDITS

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