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Physicists discover a novel quantum state in an elemental solid

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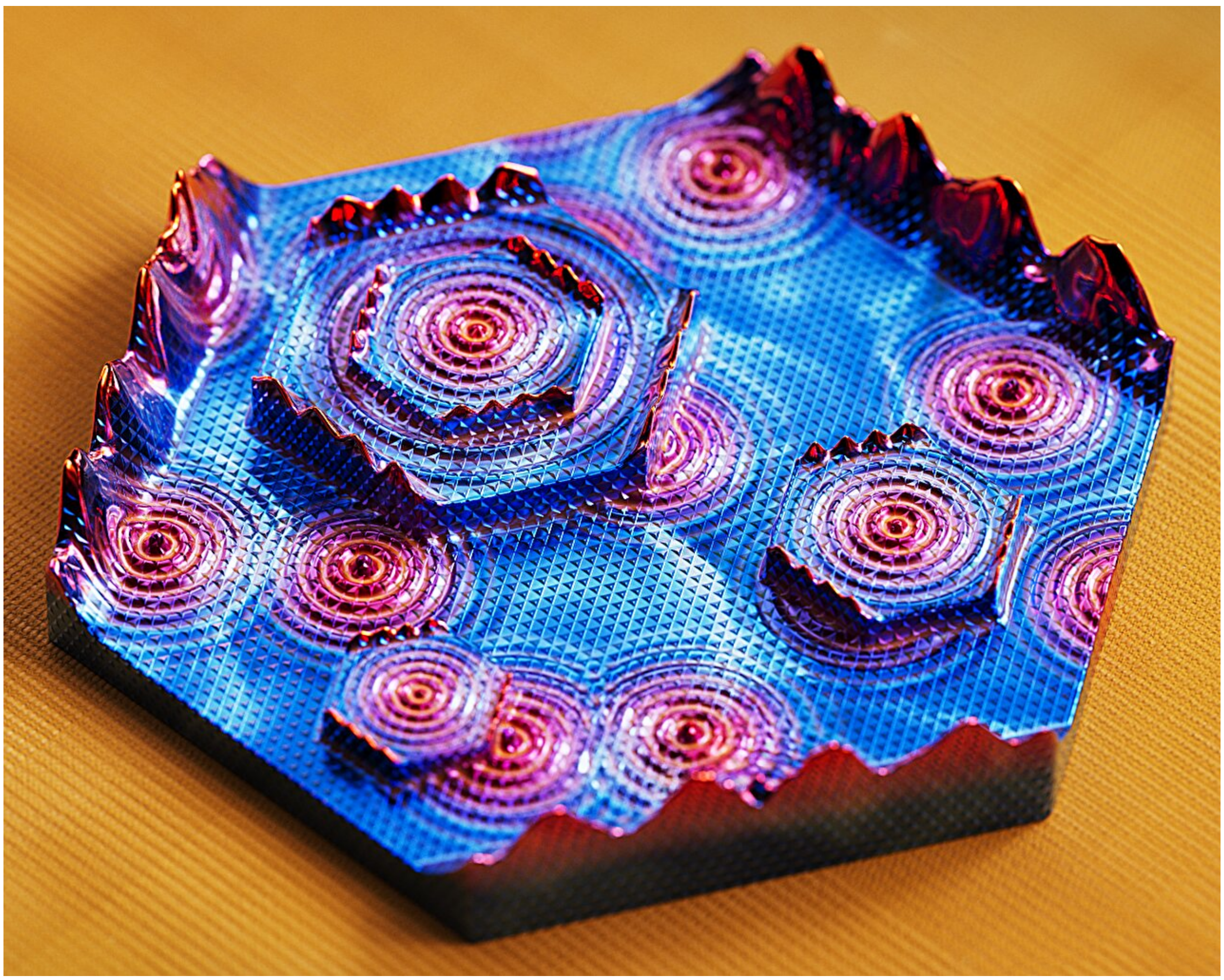

A representation of data visualization of quantum states of electrons on the surface and edge of gray arsenic crystal obtained using a scanning tunneling microscope at Princeton's physics department. Credit: Image based on STM data simulations prepared by Shafayat Hossain and the Zahid Hasan group at the Laboratory for Topological Quantum Matter at Princeton University.

Physicists have observed a novel quantum effect termed "hybrid topology" in a crystalline material. This finding opens up a new range of possibilities for the development of efficient materials and technologies for next-generation quantum science and engineering.

The finding, published in *Nature*, came when Princeton scientists discovered that an elemental solid crystal made of arsenic (As) atoms hosts a never-before-observed form of topological quantum behavior. They were able to explore and image this novel quantum state using a scanning tunneling microscope (STM) and photoemission spectroscopy, the latter a technique used to determine the relative energy of electrons in molecules and atoms.

This state combines, or "hybridizes," two forms of topological quantum behavior—edge states and surface states, which are two types of quantum two-dimensional electron systems. These have been observed in previous experiments, but never simultaneously in the same material where they mix to form a new state of matter.

"This finding was completely unexpected," said M. Zahid Hasan, the Eugene Higgins Professor of Physics at Princeton University, who led the research. "Nobody predicted it in theory before its observation."

In recent years, the study of topological states of matter has attracted considerable attention among physicists and engineers and is presently the focus of much international interest and research. This area of study combines quantum physics with topology—a branch of theoretical mathematics that explores geometric properties that can be deformed but not intrinsically changed.

For more than a decade, scientists have used bismuth (Bi)-based topological insulators to demonstrate and explore exotic quantum effects in bulk solids mostly by manufacturing compound materials, like mixing Bi with selenium (Se), for example. However, this experiment is the first time topological effects have been discovered in crystals made of the element As.

"The search and discovery of novel topological properties of matter have emerged as one of the most sought-after treasures in modern physics, both from a fundamental physics point of view and for finding potential applications in next-generation quantum science and engineering," said Hasan. "The discovery of this new topological state made in an elemental solid was enabled by multiple innovative experimental advances and instrumentations in our lab at Princeton."

An elemental solid serves as an invaluable experimental platform for testing various concepts of topology. Up until now, bismuth has been the only element that hosts a rich tapestry of topology, leading to two decades of intensive research activities. This is partly attributed to the material's cleanliness and the ease of synthesis. However, the current discovery of even richer topological phenomena in arsenic will potentially pave the way for new and sustained research directions.

"For the first time, we demonstrate that akin to different correlated phenomena, distinct topological orders can also interact and give rise to new and intriguing quantum phenomena," Hasan said.

A topological material is the main component used to investigate the mysteries of quantum topology. This device acts as an insulator in its interior, which means that the electrons inside are not free to move around and, therefore, do not conduct electricity.

However, the electrons on the device's edges are free to move around, meaning they are conductive. Moreover, because of the special properties of topology, the electrons flowing along the edges are not hampered by any defects or deformations. This type of device has the potential not only to improve technology but also to generate a greater understanding of matter itself by probing quantum electronic properties.

Hasan noted that there is much interest in using topological materials for practical applications. But two important advances need to happen before this can be realized. First, quantum topological effects must be manifested at higher temperatures. Second, simple and elemental material systems (like silicon for conventional electronics) that can host topological phenomena need to be found.

"In our labs, we have efforts in both directions—we are searching for simpler materials systems with ease of fabrication where essential topological effects can be found," said Hasan. "We are also searching for how these effects can be made to survive at room temperature."

Background of the experiment

The discovery's roots lie in the workings of the quantum Hall effect—a form of topological effect that was the subject of the Nobel Prize in Physics in 1985. Since that time, topological phases have been studied, and many new classes of quantum materials with topological electronic structures have been found. Most notably, Daniel Tsui, the Arthur Legrand Doty Professor of Electrical Engineering, Emeritus, at Princeton, won the 1998 Nobel Prize in Physics for discovering the fractional quantum Hall effect.

Similarly, F. Duncan Haldane, the Eugene Higgins Professor of Physics at Princeton, won the 2016 Nobel Prize in Physics for theoretical discoveries of topological phase transitions and a type of two-dimensional (2D) topological insulator. Subsequent theoretical developments showed that topological insulators can take the form of two copies of Haldane's model based on the electron's spin-orbit interaction.

Hasan and his research team have been following in the footsteps of these researchers by investigating other aspects of topological insulators and searching for novel states of matter. This led them, in 2007, to the discovery of the first examples of three-dimensional (3D) topological insulators. Since then, Hasan and his team have been on a decade-long search for a new topological state in its simplest form that can also operate at room temperature.

"A suitable atomic chemistry and structure design coupled to first-principles theory is the crucial step to make topological insulator's speculative prediction realistic in a high-temperature setting," said Hasan.

"There are hundreds of quantum materials, and we need both intuition, experience, materials-specific calculations and intense experimental efforts to find the right material for in-depth exploration eventually. And that took us on a decade-long journey of investigating many bismuth-based materials, leading to many foundational discoveries."

The experiment

Bismuth-based materials are capable, at least in principle, of hosting a topological state of matter at high temperatures. However, these require complex materials preparation under ultra-high vacuum conditions, so the researchers decided to explore several other systems. Postdoctoral researcher Md. Shafayat Hossain suggested a crystal made of arsenic because it can be grown in a form that is cleaner than many bismuth compounds.

When Hossain and Yuxiao Jiang, a graduate student in the Hasan group, turned the STM on the arsenic sample, they were greeted with a dramatic observation—gray arsenic, a form of arsenic with a metallic appearance, harbors both topological surface states and edge states simultaneously.

"We were surprised. Gray arsenic was supposed to have only surface states. But when we examined the atomic step edges, we also found beautiful conducting edge modes," said Hossain.

"An isolated monolayer step edge should not have a gapless edge mode," added Jiang, a co-first author of the study.

This is what is seen in calculations by Frank Schindler, a postdoctoral fellow and condensed matter theorist at the Imperial College London in the United Kingdom, and Rajibul Islam, a postdoctoral researcher at the University of Alabama in Birmingham, Alabama. Both are co-first authors of the paper.

"Once an edge is placed on top of the bulk sample, the surface states hybridize with the gapped states on the edge and form a gapless state," Schindler said.

"This is the first time we have seen such a hybridization," he added.

Physically, such a gapless state on the step edge is not expected for either strong or higher-order topological insulators separately but only for hybrid materials where both kinds of quantum topology are present. This gapless state is also unlike surface or hinge states in strong and higher-order topological insulators, respectively. This meant that the experimental observation by the Princeton team immediately indicated a never-before-observed type of topological state.

David Hsieh, Chair of the Physics Division at Caltech and a researcher who was not involved in the study, pointed to the study's innovative conclusions.

"Typically, we consider the bulk band structure of a material to fall into one of several distinct topological classes, each tied to a specific type of boundary state," Hsieh said. "This work shows that certain materials can simultaneously fall into two classes. Most interestingly, the boundary states emerging from these two topologies can interact and reconstruct into a new quantum state that is more than just a superposition of its parts."

The researchers further substantiated the scanning tunneling microscopy measurements with systematic high-resolution angle-resolved photoemission spectroscopy.

"The gray As sample is very clean, and we found clear signatures of a topological surface state," said Zi-Jia Cheng, a graduate student in the Hasan group and a co-first author of the paper who performed some of the photoemission measurements.

The combination of multiple experimental techniques enabled the researchers to probe the unique bulk-surface-edge correspondence associated with the hybrid topological state—and corroborate the experimental findings.

Implications of the findings

The impact of this discovery is two-fold. The observation of the combined topological edge mode and the surface state paves the way to engineer new topological electron transport channels. This may enable the designing of new quantum information science or quantum computing devices.

The Princeton researchers demonstrated that the topological edge modes are only present along specific geometrical configurations that are compatible with the crystal's symmetries, illuminating a pathway to design various forms of future nanodevices and spin-based electronics.

From a broader perspective, society benefits when new materials and properties are discovered, Hasan said. In quantum materials, the identification of elemental solids as material platforms, such as antimony hosting a strong topology or bismuth hosting a higher-order topology, has led to the development of novel materials that have immensely benefited the field of topological materials.

"We envision that arsenic, with its unique topology, can serve as a new platform at a similar level for developing novel topological materials and quantum devices that are not currently accessible through existing platforms," Hasan said.

The Princeton group has designed and built novel experiments for the exploration of topological insulator materials for over 15 years. Between 2005 and 2007, for example, the team led by Hasan discovered topological order in a three-dimensional bismuth-antimony bulk solid, a semiconducting alloy, and related topological Dirac materials using novel experimental methods.

This led to the discovery of topological magnetic materials. Between 2014 and 2015, they discovered and developed a new class of topological materials called magnetic Weyl semimetals.

The researchers believe this finding will open the door to a whole host of future research possibilities and applications in quantum technologies, especially in so-called "green" technologies.

"Our research is a step forward in demonstrating the potential of topological materials for quantum electronics with energy-saving applications," Hasan said.

More information: M. Zahid Hasan, A hybrid topological quantum state in an elemental solid, *Nature* (2024). DOI: 10.1038/s41586-024-07203-8.
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