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Control of Novel Topological and Superconducting States of Matter (Postprint)

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Abstract

The manipulation of material states constitutes one of the crucial driving forces behind scientific and technological advancement. Throughout human history, the control of electrons in silicon-based materials has led to the emergence of transistors and other electronic devices, ushering in the information age. However, since the advent of the 21st century, the continuous reduction in device dimensions has given rise to fundamental obstacles—such as power consumption issues, quantum tunneling, and quantum fluctuation effects—that impede further miniaturization and integration of devices, thereby creating bottlenecks for the development of modern information and electronic technologies. There is an urgent need to explore and develop a new generation of devices characterized by high efficiency, low energy consumption, and the ability to transcend quantum size effects. From a fundamental physics perspective, the physical basis of conventional semiconductor devices lies in the diffusive transport phenomenon of electrons within semiconductors. It can be argued that a profound understanding of electron diffusive transport in semiconductors catalyzed the series of information industry revolutions during the latter half of the 20th century. Consequently, overcoming the current developmental bottlenecks in the electronics industry must also be founded upon a deep understanding of electron motion patterns in novel materials and new states of condensed matter.

Full Text

Preamble

Strategic Priority Research Program (Category B) of the Chinese Academy of Sciences
Topological and Superconducting New Quantum State Manipulation

1. Background and Significance

The manipulation of material states represents a crucial driving force for scientific and technological advancement. Throughout human history, the control of electrons in silicon-based materials led to the invention of transistors and ushered in the information age. However, since the beginning of the 21st century, as device dimensions continue to shrink, fundamental issues such as energy consumption, quantum tunneling, and quantum fluctuation effects have created bottlenecks for further miniaturization and integration, hindering the development of modern information and electronic technologies. There is an urgent need to explore and develop a new generation of devices featuring high efficiency, low energy consumption, and breakthrough capabilities beyond quantum size effects.

Fundamentally, the physical basis of traditional semiconductor devices rests on the diffusive transport phenomena of electrons in semiconductors. It can be said that the profound understanding of electron diffusive transport in semiconductors catalyzed the information industry revolution of the latter half of the 20th century. Therefore, to overcome current bottlenecks in electronics development, we must achieve a deep understanding of electron motion patterns in novel condensed matter materials and new quantum states. The electromagnetic properties of materials are primarily determined by low-energy electrons near the Fermi surface. Electrons possess three degrees of freedom: charge, spin, and orbital. Transport based on spin and orbital degrees of freedom offers characteristics such as low energy consumption and high efficiency. Only by fully utilizing all three electronic degrees of freedom, seeking new quantum states, discovering novel effects, and achieving their manipulation can we break through the limitations of conventional semiconductors that rely solely on charge control, thereby fundamentally addressing the major challenges facing contemporary science and technology.

Over the past three decades, a series of important new quantum states and phenomena based on the three electronic degrees of freedom have been discovered successively, including the quantum Hall effect, topological insulators, copper-based/iron-based high-temperature superconductors, and multiferroics. Meanwhile, more than ten Nobel Prizes have been awarded for discoveries of new quantum states and effects.

The three research directions established under the "Topological and Superconducting New Quantum State Manipulation" Strategic Priority Program are firmly grounded in the three electronic degrees of freedom: (1) topological quantum state and novel quantum phenomenon research; (2) new material exploration and property studies with the long-term vision of discovering room-temperature superconductivity; and (3) exploration and manipulation of new quantum states and the design and fabrication of quantum devices. The first two directions focus on exploring new materials, new quantum states, and novel phenomena, while the third emphasizes the manipulation of new quantum states and the design and preparation of quantum devices.

Through the implementation of this program, we aim to discover 2-3 new quantum states or effects, identify 2-3 new types of unconventional superconductors, and provide several decisive experimental evidences to resolve the mechanism of high-temperature superconductivity. Simultaneously, we seek to develop new quantum state manipulation techniques, design and fabricate 1-2 prototype topological and superconducting devices, and advance novel quantum state control technologies. Through long-term stable support from this program, we hope to cultivate a cohort of internationally leading scientists, establish an international research center, guide the development direction of international topology, superconductivity, and new quantum state manipulation fields, achieve major breakthroughs, and occupy the international high ground.

2. Progress Achieved

The program has implemented an innovative R&D model of "theoretical prediction + material preparation + property measurement," positioning itself at the international forefront of basic research. By fully utilizing the charge, spin, and orbital degrees of freedom of electrons, the program has achieved a series of major original scientific results in the fields of topology, superconductivity, and new quantum state manipulation. These include the first discovery of a completely new quantum state—topological semimetals (Dirac/Weyl), the first realization of Cr-based and Mn-based compound superconductors, the first acquisition of the electronic phase diagram for the only spinel-structured oxide superconductor, the discovery of the electronic structural signature of unconventional high-temperature superconductors, the observation of Majorana fermion-like excitations in iron-based superconductors, the experimental realization of long-anticipated borophene, and the first discovery of cubic perovskite multiferroicity, among others.

During the first two years, the program published over 400 SCI papers, including 1 in *Science*, 1 in *Nature*, 14 in *Nature Communications*, 1 in *Nature Materials*, 3 in *Nature Physics*, 4 in *J. Am. Chem. Soc.*, and 20 in *Phys. Rev. Lett.* The program also applied for and was granted dozens of patents. Multiple researchers received important domestic and international science and technology awards, such as the Matthias Prize (the highest honor in the international superconducting materials field), the TWAS Physics Award, and the Second Prize of the National Natural Science Award.

2.1 Theoretical Prediction and Experimental Verification of Weyl Semimetals

Weyl semimetals feature linearly dispersive quasiparticle excitations that are topologically protected in three-dimensional bulk systems and possess definite chirality. In crystals with higher symmetry, two Weyl fermions with opposite chirality can superimpose to form a Dirac fermion state.

The program’ s Fang Zhong research team theoretically predicted in 2012 and 2013 that Na Bi and Cd As are Dirac semimetals whose Fermi surfaces consist of fourfold-degenerate Dirac points representing massless Dirac fermions. In 2014, through collaboration with international teams, they observed for the first time the theoretically predicted three-dimensional Dirac cone in Na Bi [Figure 1: see original paper]. The paper was published in *Science* and was reported by *Physics World* under the title “Scientists Discover 3D Version of Graphene” and by *Nature News* with the headline “The Wonder of Planar Physics Found in Three Dimensions.” Subsequently, they experimentally confirmed that Cd As is also a three-dimensional Dirac semimetal, with results published in *Nature Materials* in 2014. Since then, numerous experimental and theoretical works have rapidly emerged, forming a current research hotspot in condensed matter physics.

By the end of 2014, the program’ s Fang Zhong team, through first-principles calculations, theoretically predicted for the first time that the TaAs family of materials are Weyl semimetals. Unlike previous theoretical predictions, materials such as TaAs realize Weyl electronic states by breaking spatial inversion symmetry and do not require delicate and complex tuning such as doping, which facilitates experimental verification. This result immediately attracted significant attention from experimental physicists, with many research groups beginning competitive experimental verification efforts.

Specifically, the program’ s Chen Genfu team first prepared high-quality TaAs crystals, and the Ding Hong team immediately performed high-precision measurements of the electronic states on the TaAs (001) surface using the “Dreamline” ARPES experimental station at the Shanghai Synchrotron Radiation Facility. Combined with first-principles calculation results, they confirmed the existence of surface Fermi arcs [Figure 2: see original paper], providing direct experimental evidence for the Weyl electronic states in TaAs materials. By measuring bulk electronic states, they directly observed Weyl points and their associated three-dimensional Dirac cones, providing further experimental evidence. Concurrently, through precise electrical transport measurements, the Chen Genfu team observed for the first time the negative magnetoresistance effect caused by chiral anomaly in TaAs single crystals, further proving the existence of Weyl fermions from a transport perspective. The Lü Li team provided substantial assistance during this experimental process.

Subsequently, the Ding Hong, Fang Zhong, and Chen Genfu teams, along with their collaborators at the Swiss Light Source, achieved another breakthrough in this field. They conducted high-precision spin-resolved angle-resolved photoemission spectroscopy (SARPES) measurements on TaAs single crystal samples, confirming that the surface state Fermi arcs are spin-polarized.

This marks the first realization of Weyl electronic states in condensed matter and observation of their unique physical properties since Weyl fermions were proposed in 1929, holding extremely important physical significance. The discovery of Weyl semimetals not only raises many new scientific questions but also brings hope for future revolutionary technological breakthroughs. In Weyl semimetals, due to topological protection, scattering between two Weyl electronic states with opposite chirality is weak, which can be utilized to achieve extremely low-energy electronic transport. Particularly, these electronic states can exist stably at room temperature, which is of great value for room-temperature low-power electronics applications. Currently, an international research boom on TaAs family materials has emerged. Our work on theoretically predicting and experimentally verifying Weyl fermions in TaAs was completed independently and simultaneously with related work by Princeton University, receiving widespread recognition and high praise from the international academic community. This achievement was selected as one of "Physics World' s Top 10 Breakthroughs of 2015," as an "Iconic Advance" by the American Physical Society (APS) in 2015, and as one of China' s Top 10 Scientific Advances of 2015 by the Ministry of Science and Technology.

2.2 First Discovery of Superconductivity in Cr-Based and Mn-Based Compounds

3d transition metal compounds exhibit extremely rich quantum states and novel quantum phenomena, including magnetic ordering, giant magnetoresistance, spin and charge density waves, metal-insulator transitions, multiferroicity, and superconductivity. Among these properties, unconventional high-temperature superconductivity in copper-based and iron-based compounds represents one of the core research topics in condensed matter physics. Among the 3d elements in the periodic table, all elements except Cr and Mn have superconducting compounds. Exploring Cr- and Mn-based superconducting materials, particularly unconventional superconductivity, has long been an important focus in superconducting materials and physics research.

The program' s Luo Jianlin research group, Cheng Jinguang research group, Jin Changqing research group, and collaborators including Professor Yoshiya Uwatoko from the University of Tokyo discovered superconductivity in CrAs under high pressure, realizing the first Cr-based compound superconductor. They also found that its normal state exhibits non-Fermi liquid behavior, suggesting possible unconventional superconductivity.

Building on this work, the Cheng Jinguang research group, Luo Jianlin research group, and Yoshiya Uwatoko' s team from the University of Tokyo collaborated to achieve for the first time a high-pressure-induced magnetic quantum critical point and observe superconductivity in MnP [Figure 3: see original paper], thereby realizing the first Mn-based compound superconductor. This represents an important advance in the exploration of superconductors among 3d transition metal compounds and breaks the previous consensus that Mn-containing compounds cannot be superconducting. This work was published in *Physical Review Letters* and selected as an Editors' Suggestion. Meanwhile, Michael R. Norman from Argonne National Laboratory wrote a dedicated Viewpoint in *Physics* commenting on this work, noting that the discovery of superconductivity in CrAs and MnP provides important model systems for studying the relationship between helical magnetism and superconductivity, an area where research is currently very limited.

2.3 Discovery of Cubic Perovskite Magnetoelectric Multiferroic Materials

Magnetoelectric multiferroic materials simultaneously possess magnetic ordering and electric polarization ordering, enabling magnetic field control of electric polarization or electric field manipulation of magnetic properties through the coexistence and coupling of these two order parameters. Over the past decade, multiferroic materials have been a research hotspot in condensed matter physics and materials science due to their rich physical content and broad application prospects. Perovskite oxides represent one of the most important material systems for studying ferroelectricity and multiferroicity. In traditional perovskite ferroelectrics, electric polarization originates from ionic displacements that break spatial inversion symmetry. Therefore, it is generally believed that ferroelectric ordering cannot appear in high-symmetry lattices with inversion centers (such as cubic lattices). Indeed, ferroelectricity has never been observed in cubic perovskite systems. However, in multiferroic materials, the origin of electric polarization is no longer limited to ionic displacements and can have much more diverse origins, even being closely related to spin structures. Meanwhile, the total symmetry of the system is determined jointly by crystal symmetry and magnetic symmetry, not requiring each to individually break spatial inversion symmetry. Under certain special circumstances, high-symmetry cubic lattices may also exhibit electric polarization and multiferroicity. Nevertheless, until now, no real case of cubic perovskite multiferroicity has been found.

Recently, the program’ s Long Youwen team, Sun Yang team, and their collaborators achieved a breakthrough in cubic lattice multiferroicity research, discovering for the first time a cubic perovskite multiferroic material, LaMn Cr O [Figure 4: see original paper]. This research not only represents an important breakthrough in the preparation of cubic lattice multiferroic materials but also introduces entirely new physical research content. Density functional theory calculations reveal that spin-orbit coupling effects of magnetic ions play a crucial role in the emergence of electric polarization. However, existing theoretical models for multiferroicity originating from magnetic ordering are insufficient to explain the microscopic origin of this special multiferroicity, necessitating the development of entirely new theoretical models. Furthermore, since there is no contribution from ionic displacements, the electric polarization in this system may be generated entirely by electron cloud distortion, making LaMn Cr O a typical example for studying novel electronic ferroelectrics. Further in-depth investigation into the origin of cubic perovskite multiferroicity and magnetoelectric coupling mechanisms may have important impacts on the exploration of new multiferroic materials and the study of new physical mechanisms. The related research results were recently published in *Physical Review Letters* and selected as a PRL Editors' Suggestion, while also being highlighted by the American Physical Society website' s news commentary section *Physics* under the title "Multiferroic Surprise."

3. Originality

(1) In topological state research, most of the novel quantum effects we aim to study have never been realized experimentally. Their realization would produce unprecedented advances in fundamental condensed matter physics and information technology. All research topics directly target the realization of quantum effects, with material prediction, design, selection, and preparation methods all considering how to more easily achieve and observe various quantum effects. Close integration of material design, material preparation, atomic and electronic structure characterization, device fabrication, and quantum effect observation facilitates rapid identification of key factors affecting the emergence of quantum effects.

(2) In superconductivity research, we combine multiple aspects including new material exploration, property studies, and mechanism investigations. By fully leveraging the unique advantages of the Chinese Academy of Sciences' large scientific facilities, various advanced spectrometers, and a strong talent pool with accumulated experience, we maintain close collaboration and integration to continuously strive toward revealing the physical essence of novel quantum states in unconventional superconductors. Meanwhile, the close combination of experiment, theory, and computation not only enables full theoretical interpretation of experimental results but also enhances our ability to tune multiple physical parameters, design original key experiments, and discover more new superconducting materials, continuously advancing toward the long-term goal of room-temperature superconductivity.

(3) In new quantum state manipulation and device exploration, the discovery of topological superconductors and Majorana fermions represents major breakthroughs in this field. Additionally, in new device development, magnetoelectric multistate memory devices are inherently innovative. Although memory devices utilizing either ferroelectric or ferromagnetic properties separately have been applied, multistate memory devices simultaneously employing both ferroelectric and ferromagnetic domains have not yet been reported. Novel ferroelectric resistance memory can overcome the stability issues of conventional resistance memory and the destructive read-write problems of traditional ferroelectric memory, while inheriting the advantages of both. Moreover, its storage density can be substantially increased compared to traditional ferroelectric or ferromagnetic memory devices. Therefore, the innovation in new device development under this program lies in the simultaneous utilization of both magnetic domain and electric domain polarization states for novel magnetoelectric multistate memory devices, based on the manipulation of quantum states and mag-

netoelectric properties in low-dimensional transition metal oxides.

4. Significance for Industry

While conducting frontier basic research, this program actively explores applied basic research, investigates new quantum state manipulation, and develops high-efficiency, low-power consumption, multifunctional prototype devices. This work lays the scientific foundation for future disruptive technological innovations such as low-power computer chips, lossless power transmission, topological quantum computers, and environmentally friendly thermoelectric and magnetoelectric materials and devices, thereby promoting the emergence of strategic emerging industries. In the program' s research on novel semiconductor devices, we have developed composite metal substrate technology suitable for high-reflectivity flexible applications and further advanced high-end semiconductor LED technology, which is highly beneficial for LED industry upgrading and resource conservation.

5. Recommendations for Future Development in Disciplines, Industry Promotion, and Talent Cultivation

We recommend strengthening basic research and forward-looking deployment to promote comprehensive development of scientific research, talent cultivation, and platform construction. We should adhere to a people-centered approach, vigorously create an environment and culture conducive to innovation, and enhance China' s original innovation capabilities. We should explore new organizational models for basic research and improve mechanisms combining stable support with competitive selection. For major projects, excellent teams, and key platforms that have undergone scientific demonstration, sustained and stable support should be provided, allowing scientists to focus their main time and energy on scientific research and diligent investigation.

We should conduct basic research with distinctive features and advantages in line with national objectives, industry development directions, and regional development needs to enhance future industry competitiveness, public service levels, and regional innovation capabilities. We should innovate the technology transfer and transformation mechanisms for basic research achievements, promote deep cooperation among industry, academia, and research institutes, and enable basic research to better contribute to society.

(Supporting Institution: Institute of Physics, Chinese Academy of Sciences)

Expert Comment 1

This is an excellent project with numerous outstanding talents working together diligently. The significant impact of this program is evident from the published papers and citation counts, but this is not the most important aspect. As mentioned in other reports, the highlight of this project is the theoretical prediction and experimental observation of topological semimetals. The topological stability that can coexist with gapless bulk states represents a new mechanism, different from the well-known coexistence of topology and gapped insulators since the 1980s. These studies were completed by a few top-tier condensed matter physics research groups worldwide and represent the most original achievements in condensed matter physics research in recent years. The project leaders (particularly Fang Zhong, Dai Xi, and Ding Hong) and their colleagues have made contributions equally important as other leading research groups in this rapidly expanding field. Other research aspects are equally excellent, with more application-oriented directions such as better magnetoelectric thin films and improved superconductors, which will certainly lead to technological breakthroughs in the future.

Expert Comment 2

The research content of this program represents a very active field in condensed matter physics research, with high priority in the world' s basic research landscape and enormous prospects for technological applications. I hold this program in high regard. The program can be essentially divided into two aspects: one is basic research exploring new materials and phenomena, and the other focuses on technological applications. In my view, this is an excellent balance. The main research achievements of the program are internationally recognized, with some leading internationally. The program has produced many high-quality academic papers.

(Anonymous evaluations from international review experts for the 2016 midterm assessment of the Strategic Priority Program)

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