S 拓扑材料、物理与器件

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S001

专题代号：S

Majorana费米子的调控和编织

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摘要：Majorana费米子是由意大利物理学家Majorana于80多年前提出的一种基本粒子。它是一种很特殊的费米子，它的反粒子就是其自身。近十年来，人们在凝聚态体系中提出一些准粒子激发也具有Majorana费米子的性质，即其产生算符和湮灭算符相同，这样的准粒子服从非阿贝尔统计。由于其特殊性质，Majorana费米子在拓扑量子计算方面有重大应用前景。在该报告中，我将介绍Majorana费米子，并介绍我们在Majorana费米子领域的最近理论研究进展，包括调控Majorana费米子的相位，实现其编织和证实交换非阿贝尔特性等。

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S002

专题代号：S

Nonlinear Hall effect

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摘要：Unconventional responses upon breaking discrete or crystal symmetries open avenues for exploring emergent physical systems and materials. By breaking inversion symmetry, a nonlinear Hall signal can be observed, even in the presence of time-reversal symmetry, quite different from the conventional Hall effects. However, less is known when a strong nonlinear Hall signal can be measured, in particular, its connections with the band-structure properties. By using model analysis, we find prominent nonlinear Hall signals near tilted band anticrossings and band inversions [1]. These band signatures can be used to explain the strong nonlinear Hall effect in the recent experiments on two-dimensional WTe2 [2]. Disorder plays indispensable roles in various linear Hall effects. We derive the formulas of the nonlinear Hall conductivity in the presence of disorder scattering and construct the general scaling law of the nonlinear Hall effect, which may help in experiments to distinguish disorder-induced contributions to the nonlinear Hall effect [3].

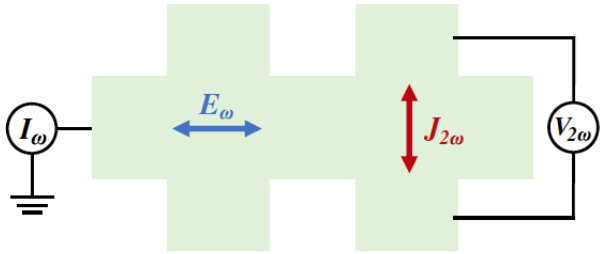

Fig. 1 Schematic of how to measure the nonlinear Hall effect in a standard Hall bar. The experimentally measured I−V relation is related to the theoretical Berry dipole defined by the electric field-current density (E−J) relation.

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S003

专题代号：S

High-Chern-Number and High-Temperature Quantum Hall Effect without Landau Levels

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摘要： The quantum Hall effect (QHE) without Landau levels (LLs) has become a long-pursuit research topic since the QHE was discovered around 40 years ago. Previous theoretical proposals and experiments based on two dimensional (2D) topological systems with time-reversal symmetry broken have revealed the QHE without LLs with Chern number C=1 at ultralow temperatures. Now the key issues of the QHE without LLs are how to increase the working temperature and realize high Chern number with more dissipationless chiral edge states (C>1) for emerging physics and low-dissipation electronics. We discovered the high Chern number (C=2) QHE without LLs in the nine-septuple-layer magnetic $MnBi_2Te_4$ nano-device and C=1 Chern insulator state in the seven-septuple-layer nano-device displaying nearly quantized Hall resistance plateau at record-high temperatures up to 60 K. [1] The thickness-dependent topological quantum phase transition from C=2 to C=1 is uncovered. To our knowledge, this is the first work to report high Chern number QHE without LLs above the liquid helium temperature and this is also the first time that the nearly quantized Hall resistance plateau is detected at the temperature up to 60 K for QHE without LLs.

关键词： Quantum Hall Effect without Landau Levels, High-Chern-Number, Chern Insulator, Quantum Anomalous Hall Effect, $MnBi_2Te_4$

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S004

专题代号：S

Recent progress in the study of topological materials Bi_4X_4 (X = I, Br)

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摘要：A wide variety of topological materials presenting intriguing states of quantum matter have mostly been discovered in two-dimensional and three-dimensional systems. Very recently, a novel quasi-one-dimensional family of bismuth halogenides, Bi_4X_4 (X = I, Br), has attracted considerable attention because it can be easily tuned by external pressure and cleaved in practical applications. Here, based on our theoretical predictions and experimental observations, we give a brief progress report on the study of these materials which exhibit rich phase diagrams and novel properties, including strong/weak topological insulators, composite Weyl semimetals, and Infrared absorption of the topologically originated edge states as well as pressure-induced superconductive and structural phase transitions [1-6]. These findings provide critically valuable information to understand the physics behind the new topological phenomena.

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S005

专题代号：S

拓扑半金属-超导体异质结

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摘要：本报告将汇报我们在拓扑半金属纳米结构及其与超导体构成的异质结中的量子输运方面的工作，具体包括：外尔费米子手征反常导致的负磁电阻效应[1]，以及反常的磁热电效应[2]；起源于拓扑表面态输运的π A-B效应[3]，连续体态和离散表面态耦合产生的Fano共振现象[4]，以及拓扑表面态的量子Hall效应[5]；狄拉克半金属-超导体约瑟夫森结中超导临界电流的Fabry-Pe´rot (F-P)振荡[6]，以及4π周期的超导电流以及Majorana费米子零能模[7]。这些工作为低维材料中量子态调控与新型信息器件提供了新思路。

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S006

专题代号：S

Routes to quantum anomalous Hall effect from superlattice-like magnetic topological insulators

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摘要：As one of paradigmatic phenomena in condensed matter physics, the quantum anomalous Hall effect (QAHE) in stoichiometric Chern insulators has drawn great interest for years. Recently, $MnBi_2Te_4$ thin films manifests the QAH effect at a record high temperature of 4.5 K in the forced ferromagnetic state above 10 Tesla. By realizing a bulk $MnBi_4Te_7$ with alternating $[MnBi_2Te_4]$ and $[Bi_2Te_3]$ layers, we suggest that it is a Z_2 antiferromagnetic topological insulator with a small out-of-plane saturation field of ~ 0.2 Tesla. Using model Hamiltonian analysis and first-principle calculations, we then establish a topological phase diagram and map on it with different two-dimensional configurations, which is taken from the recently-grown magnetic topological insulators $MnBi_4Te_7$ and $MnBi_6Te_{10}$. These configurations manifest various topological phases, including quantum spin Hall effect with and without time-reversal symmetry, as well as QAHE. We then provide design principles to trigger QAHE by tuning experimentally accessible knobs, such as slab thickness and magnetization. Our work reveals that superlattice-like magnetic topological insulators with tunable exchange interaction serve as an ideal platform to realize the long-sought QAHE in pristine compounds.

S007

专题代号：S

石墨烯体系中拓扑边界态（拓扑导电通道）研究

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摘要：在本报告中，我将简要介绍我们课题组在石墨烯中可能出现的几种拓扑边界态和拓扑导电通道的研究进展，包括垂直外磁场作用下量子霍尔边界态，双层石墨烯AB-BA畴界的拓扑导电通道，双层小转角石墨烯体系中的拓扑导电通道网络，应变石墨烯中可能出现的量子谷霍尔效应和谷极化的量子霍尔效应，单层石墨烯量子霍尔铁磁态中可能实现的量子自旋霍尔边界态等。

S008

专题代号：S

Topological Crystalline Insulators with C2 Rotation Anomaly

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摘要：Symmetry protected topology has been largely extended from time-reversal symmetry to crystalline symmetries [1]. Based on the topological quantum chemistry theory [2] or symmetry-based indicators [3], the band topology has been related with the localized atomic orbitals in chemistry picture and the topological nontrivial state can be identified from the trivial atomic insulators by examining their symmetry data. In addition to the well-known topological crystalline insulators protected by mirror or glide symmetry, those protected by rotation, screw, inversion and S4 symmetries have also been found. [4, 5, 6] We have proposed two candidate compounds, also listed in the three topological materials databases [7, 8, 9], can host the topological crystalline insulators protected by C2 rotational symmetry and C2 screw symmetry, respectively. Both of them have two helical hinge states related by the C2 rotation. The former has two Dirac cones at generic momenta on the surface perpendicular to C2 rotation axis, while the later does not have. We developed a method based on Wilson loop technique to prove the existence of these surface Dirac cones due to C2 anomaly and precisely locate them as demonstrated.

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S009

专题代号：S

Static and dynamical axion states in magnetic topological materials

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摘要：Axion is a hypothetical elementary particle which was postulated to solve the charge conjugation parity problem in the Standard Model of particle physics. However, axion has not yet been observed in nature and remains mysterious. Interestingly, the axion field emerges in effective theory of topological insulators and attracts extensive attention in condensed matter physics. The time-reversal and inversion symmetries constrain the axion field to be quantized. Once the time-reversal and inversion symmetries are broken, the axion field becomes dynamical along with magnetic fluctuations, so-called the dynamical axion field. In this talk, we will talk about quantized (static) and dynamical axion states in magnetic topological insulators and their novel physical properties.

关键词：静态轴子态，动态轴子态，量子磁电耦合，赝自旋陈数

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S010

专题代号：S

四维拓扑绝缘态及其在电路中的实现

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摘要：拓扑态可以存在于维度高于三维的物理系统。它们具有新奇的边界态和特殊的拓扑响应，却难以在凝聚态体系中实现。 近期研究表明，在光子晶体和电路网格等人工系统中容易实现这类高维度的能带结构。此次报告将介绍如何设计四维的AI类拓扑绝缘体。我们先给出一个拓扑非平庸的最简模型，其拓扑数由第二陈数描述。然后介绍如何在电路网络中实现此四维拓扑态。由于电路的具体性质只与器件的拓扑连接方式相关，我们可以把这个四维网络投影到一个二维电路板上，方便在实验上实现。我们建立了电路的基尔霍夫方程和四维拓扑态哈密顿量的对应关系，并用电路仿真软件检验了电路的谐振频谱。我们发现在四维系统的三维边界上，其谐振频谱呈现出一对手性相同的三维外尔态，这是四维拓扑非平庸态的一个显著标志。这些拓扑性质可以通过测量电路结点上的电压信号而获得，在实验上非常简单易行。

关键词：四维拓扑绝缘体, 拓扑电路

参考文献 ：R Yu, YX Zhao, AP Schnyder， A genuine realization of the spinless 4D topological insulator by electric circuits， arXiv:1906.00883

S011

专题代号：S

Topological aspects and optical properties of twisted bilayer and multilayer graphene systems

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摘要：In this talk we discuss the electronic structures, topological properties, and optical properties of twisted bilayer and multilayer graphene systems. We propose that the two low-energy flat bands in twisted bilayer graphene (TBG) are equivalent to two zeroth pseudo Landau levels with opposite sublattice polarizations and carry opposite Chern numbers +/-1. Such a pseudo Landau-level representation of TBG naturally explains the origin of ``magic angles'' in TBG, and have significant implications on the nature of the correlated insulating phases observed in experiments. The pseudo Landau-level representation can be further generalized to twisted multilayer graphene (TMG) systems, in which a universal valley Chern-number hierarchy can be derived for the two low-energy flat bands of the system. The nontrivial Chern numbers in the TMG systems are associated with large and valley contrasting orbital magnetizations, which generate circulating current loops and local magnetic field distributions on the moire scale, which can be experimentally detected. We propose that the topologically nontrivial bandstructures in TBG and TMG can be probed by both magneto-optical Kerr/Faraday rotations, as well as nonlinear optical responses such as shift currents and second harmonic generation.

关键词：twisted graphene, band topology, Landau levels, optical properties

S012

专题代号：S

Three-dimensional quantum Hall effect in $ZrTe_5$

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摘要：The discovery of quantum Hall effect had greatly improved the understanding of the phase transitions and topological orders in two-dimentional systems. It is natural to ask whether there are similar phemomena that might occur in three-dimentional gas systems. However, the long-sought three-dimensional (3D) quantum Hall effect has not been well experimentally demonstrated in 3D gas system. Here we report an experimental observation of three-dimensional quantum Hall effect in zirconium Penta-telluride（$ZrTe_5$）within a magnetic field B (<1.3T). We also discover that each Quantum Layer contributes $2e^2/h$ with a thickness of one Fermi wavelength λ_F in b direction. As further increasing magnetic field, the system has reached the Quantum Limit regime, where the resistance $\rho_{xx}(B)$ increases dramatically and displays Metal-Insulator transition behavior. With analysing $\rho_{xx}(B)$ scaling plots, we confirm this Metal-Insulator transition is a many-body quantum topological phase transition. Our finding not only provides a new understanding of the interplay between 2D and 3D Landau quantization but also allow for the further exploration of the higher dimensional electronic gas system and exotic strongly corrected topological phase transitions.

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S013

专题代号：S

Magnetic Topological Semimetals with Kagome Lattices

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摘要： The origin of anomalous Hall effect (AHE) in magnetic materials is one of the most intriguing aspect in condensed matter physics and has been a controversial for a long time. Recent studies indicate that the intrinsic AHE is closely related to the Berry curvature of occupied electronic states. In a magnetic Weyl semimetal with broken time-reversal symmetry, there are significant contributions to Berry curvature around Weyl nodes, which would lead to a large intrinsic AHE. In addition, the real-space non-coplanar spin texture can also lead to significant AHE, so called topological Hall effect (THE). On the other hand, the kagome lattice is known to host exotic quantum magnetic states. Theoretical work has predicted that kagome lattices may also host topological electronic states. In this presentation, we introduce several kinds of materials, such as Fe_3Sn_2, $Co_3Sn_2S_2$ and YMn_6Sn_6 with Kagome lattice, which show large AHE and THE, and it can be ascribed to the existence of Weyl or Dirac fermions in these systems as well as the real-space spin texture. It indicates that magnetic kagome metals provide a new platform to study on the emergent topological electronic properties in a correlated electron system.

S014

专题代号：S

Microscopic theory of in-plane critical field in two-dimensional Ising **superconducting systems**

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摘要：I will show our theoretical attempts to study the in-plane critical magnetic field of two-dimensional Ising superconducting systems, and to propose the microscopic theory for these systems with or without inversion symmetry[1]. Protected by certain specific spin-orbital interaction which polarizes the electron spin to the out-of-plane direction, the in-plane critical fields largely surpass the Pauli limit and show remarkable up-turn in the zero temperature limit. The impurity scattering and Rashba spin orbital scattering, treated on equal-footing in the microscopic framework, both weaken the critical field but in qualitatively different manners. The microscopic theory is consistent with recent experimental results in Pb[2,3] and stanine[4] superconducting ultra-thin films.

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S015

专题代号：S

Defect Engineering on Monolayer MoS_2 for 2D Electronics and Optoelectronics

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摘要： Emerging two-dimensional (2D) materials represented by ultrathin MoS_2 have been considered ideal alternatives for next-generation circuits because of their atomic-level thickness, superior theoretical mobility, moderate band gap, and stable structure. Unlike silicon, ultrathin, especially monolayer, MoS_2 logic units are difficult to construct through silicon-based doping schemes (atomic substitution and ion implantation) because the ultrathin body is prone to lattice disruption and doping instability. Nevertheless, defects, which customarily act as negative components, may play a stable and positive role in modulating the electronic structure of MoS_2 to build atomically thin logic devices. Defects in MoS_2 need to be precisely controlled before they can be of value. Furthermore, to build logic devices, most of the existing defect-controlling technologies are not sufficiently compatible with complementary metal-oxide-semiconductor (CMOS) processes. In addition, complex technology, high cost, and limited implementation scope restrict the application of defect modulation in the field of ultrathin MoS_2 circuits.

Here, I will introduced our strategies for the construction of an atomically thin MoS_2 opto- and electronics by defect engineering. According to the defect engineering, the modulation of electronic structure, the optimization of contact resistance, and the strong interlayer coupling effect have been observed, which could be benefit to the construction of monolayer and bilayer homogeneous opto-electronics and logic electronics.

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S016

专题代号：S

携带拓扑核的能带简并

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摘要：外尔点是三维空间中携带拓扑核的零维能带简并点。拓扑核的存在使简并点免于微扰影响而解简并，并且能够产生各种有趣的物理现象，如拓扑保护的负折射现象。值得注意的是，除了外尔点之外，还存在携带拓扑核的更高维度的能带简并。在这里，我们引入带拓扑核的能带节面（Nodal Surface）和节线（Nodal Line）的概念。在动量空间中携带拓扑核的二维能带简并面（一维能带简并线），我们称之为带核节面（带核节线）。我们首先给出了这一类带核节面和节线的有效哈密顿量，并进一步提出紧束缚模型以及声学超材料来实现这一类能带结构。利用声子晶体，我们已经实验上观测到了带拓扑核的节面。实验测量到的拓扑保护表面“费米弧”与仿真模拟结果符合得很好。与外尔拓扑半金属不同，拥有拓扑核节面/节线系统的表面“费米弧”连接外尔点与节面/节线的投影。更重要的是，“费米弧”与节面/节线投影位置的连接点极度依赖于边界条件。而在带拓扑核节线系统中，我们发现表面态呈电扇页形状分布而非常见的鼓膜分布。另外有趣的是，在节面半金属系统中，节面通过“吸收”或“释放”外尔点使节面的带核属性发生改变，从而实现拓扑相变。我们的研究表明，在能带理论中，携带拓扑核的能带简并不仅仅只有零维的点（如外尔点），这为拓扑材料的设计提供了更多可能。

关键词：外尔半金属，带核节面/节线，拓扑半金属，拓扑核

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S017

专题代号：S

First-principles Studies of Periodically Driven Quantum Materials

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摘要： Recent advances in ultrafast spectroscopy open a route toward engineering new phase of solids with optical pumping. The nonequilibrium electronic states of solids driven by the electromagnetic field manifest novel topological states which don't exist at equilibrium conditions. Using first-principles calculations and Floquet theorem, we studied the dressed states of some quantum materials including black phosphorous and graphene under periodic driving of laser. Intriguing photo-dressed electronic states including Floquet Dirac semimetals, Floquet topological insulators *etc* can be engineered in black phosphorous by changing the direction, intensity and frequency of incident laser [1]. In the transition boundary between type-I and –II FDF, we found one critical type-III FDF, which could be utilized to achieve the highest Hawking temperature T_H hitherto reported [2]. The real-time tracking of the dynamic topological phase transition in type-II Weyl semimetal $WeTe_2$ is also obtained by time-dependent density functional theory (TDDFT). The pair of Weyl points can be annihilated by light illumination, and stabilized as well [3]. Our works demonstrate examples of the nonequilibrium topological states of two-dimensional materials by first-principles calculations, and open an avenue towards the coherent control of electron dynamics of quasiparticles, and Floquet engineering of quantum materials.

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[1] H. Liu *et al*., *Phys. Rev. Lett*. 2018, 120, 237403.

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[3] M. X. Guan, et al., Unpublished.

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S018

专题代号：S

The Geometry of Electromagnetic Multipoles

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摘要：There is no historical evidence confirming that Henri Poincaré ever met Gustaev Mie, but what would happen if the two contemporary polymaths come face to face? Our work would allow us to conjecture that Henri Poincaré, after knowing the Mie scattering theory, would probably make a comment like this: Multipoles are like people, it is their imperfections that make them interesting.

Electromagnetic multipoles have been serving as a fundamental language spanning different branches of optics and photonics. Their general features including radiation patterns and polarization distributions have been indelibly planted in the brains of physicists, while in sharp contrast rarely anybody cares about directions along which there are no radiations, as they naturally have been taken for granted to be trivial.

Here we reapproach electromagnetic multipoles from a topological perspective and discover there is actually “more light” in the darkness. Those dark directions essentially correspond to singularities (zeros) of the corresponding tangent vectorial fields, which can be generally categorized by their Poincaré indexes In this work, we provide exhaustive maps for all multipoles, which pinpoint their singularities, specify the indexes, and show that the index sum across the entire momentum sphere is always 2, agreeing with the Poincaré-Hopf theorem. Based on those revealed topological features of multipolar radiations, we come up with a novel multipolar reinterpretation for bound states in the continuum: their formation originates from the overlapping of multipolar singularities with allowed open radiation channels. This revelation subtly connects the indexes of multipolar singularities to topological charges of those bound states, showing that they are fundamentally equivalent.

Our work have fused two central and sweeping concepts of multipoles and topologies. Considering the ubiquitous roles of electromagnetic multipoles throughout photonics, this work can accelerate the pervasion of topological concepts into more optical branches. Furthermore, multipoles broadly serve as a fundamental tool and language for many other fields in physics and interdisciplinary studies involving wave effects, on which our work generally shed new light from a more fundamental topological perspective.

关键词： Electromagnetic Multipoles; Mie Theory; Singularities; Bloch Modes.

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S019

专题代号：S

拓扑节线半金属 ZrSiSe 中的“半缺失”Umklapp 散射

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摘要：ZrSiSe 是 2017 年被实验验证的新一代拓扑半金属—狄拉克节线半金属的代表材料，其晶体结构具有的非点式空间群（nonsymmorphic spacegroup），这决定了其表面必然存浮动带型非传统表面态。然而，无论理论还是实验，对该类型表面态具备什么样的非常规物理性质都基本一无所知。

我们通过单缺陷的准粒子干涉技术分别对 ZrSiSe 晶体（001）面上单个 Si 缺陷和 Zr 缺陷进行测量。首先在四重对称性的晶体表面发现具有二重干涉信号的 Si 缺陷，并且随着能量增加恢复四重对称性。其次在 Zr 缺陷上发现违反传统倒逆散射定义的“半缺失”Umklapp 散射，结合计算和理论分析，发现该效应源于其晶体结构的非点式对称性产生的浮动带表面态，并适用于具有非点式对称性晶体结构的材料。

关键词：拓扑半金属，扫描隧道显微镜

S020

专题代号：S

光子晶体平板中拐角模式的实验观测

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摘要：近年来，科学家提出基于二维Su-Schrieffer-Heeger模型的拓扑光子晶体，它支持零维受拓扑保护的拐角模式。为了实现对拐角模式的观察，我们设计了以完美电导体作为衬底的光子晶体平板结构。首先，该光子晶体平板结构使得实验测量过程中无需在样品上方加盖金属板，为直接探测样品的本征模式提供了有利条件。其次，完美电导体的镜像作用使得介质柱等效高度增大为实际高度的两倍，有效地降低了实验中所需材料的高度。另外，完美电导体施加的边界条件能够抑制类横电偏振模式，消除了这些模式对实验测量的影响。基于该新型光子晶体平板结构，我们研究原胞由四根介质柱组成的光子晶体平板结构。通过调整四根介质柱的间距，发现了二维扎克相位的拓扑相变过程。根据二维扎克相位的不同，我们可以理论预言光子晶体平板的边界模式和拐角模式。在微波实验中，我们利用近场扫描平台对的边界模式和拐角模式进行了直接成像，为理论预言结论提供了有力的实验证据。进一步地，我们还在硅基平板结构中实现了近红外频段的拐角模式的实验观测。光子晶体平板中的拐角模式为诸如高品质因子腔模等新型光场调控提供了设计新思路，同时在增强光学非线性效应、片上激光光源和光学传感等方面也具有潜在的应用前景。

关键词：拓扑光子学、光子晶体平板、光场调控、微纳光子学

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S021

专题代号：S

拓扑狄拉克半金属中的三维量子霍尔效应

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摘要：狄拉克半金属是一种新型拓扑量子材料，受晶格对称性保护，其能带上具有简并的狄拉克锥结构，被称为“三维石墨烯”。狄拉克半金属可作为一系列其它新奇量子态的母体材料，在某些对称性被打破的情况下，体系会相应演化成拓扑绝缘体、外尔半金属和拓扑超导体等。进一步研究这些对称性破缺诱导的相变能使人们对拓扑量子材料有更为深刻的认识，由于三维狄拉克半金属在高维度拓扑材料、拓扑相变等基础领域和量子计算、高迁移率导电材料、磁感应器等应用方面的前景，国际上已经兴起一场关于狄拉克半金属的研究热潮。本次报告将着重介绍拓扑半金属的重要特征-费米弧表面态以及由上下表面费米弧耦合起来形成的外尔轨道。实验中利用楔形样品实现可控的厚度变化，这样外尔轨道在不同厚度区域发生隧穿所需时间不同，导致对应轨道状态发生变化。通过测量对应的量子霍尔电阻，实验发现回旋轨道能量能直接受到样品厚度的调控，和常规的基于二维表面态的量子霍尔效应完全不同。同时，改变磁场方向，发现轨道能量也受到磁场和晶向的相对位置的影响，打破了二维体系应该具有的镜面对称性。基于这两个重要证据，实验成功证明了砷化镉纳米结构中的量子霍尔效应来源于三维的外尔轨道【1-2】。三维量子霍尔效应的实现打破了维度限制，这一发现为未来三维空间电子的量子化传输提供了新的思路和实验基础。

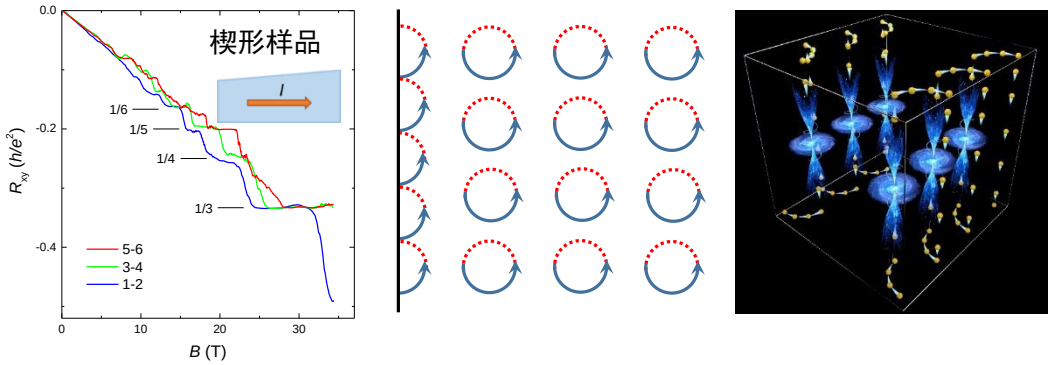

图 1 砷化镉中的三维量子霍尔效应及示意图【1-2】

关键词：三维量子霍尔效应，狄拉克半金属，强磁场

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资助项目：国家自然科学基金（11474058, 11874116, 61674040）

S022

专题代号：S

中子散射对拓扑磁振子与拓扑材料声子的研究

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在本报告中，我将介绍我们最近在运用非弹性中子散射研究量子材料的磁振子、声子等元激发中所取得一些最新成果。包括：1）我们在三维反铁磁体Cu_3TeO_6中发现了材料同时存在狄拉克点与三重简并点，首次在真实材料体系中实现了三维拓扑磁振子[1]；2）通过研究拓扑超导体系$Sr_xBi_2Se_3$中的声子，发现了在长波极限下[001]方向的奇异声子。在强自旋轨道耦合的协助下，该声子能够诱导出具有强烈各向异性的强电声子耦合，从而使材料具有破坏面内旋转对称性的奇宇称超导配对，证明了电声子耦合可以诱导出非常规超导电性[2]。

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[2] Nat. Commun. 10, 2802 (2019).

S023

专题代号：S

Nonlinear optical Hall effect in topological semimetal

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We classified the sources of second harmonic generation (SHG) of the Weyl semimetal by collisionless quantum kinetic equation into three kinds: i.e., injection current from the canonical band dispersion, shift current from a gauge invariant shift vector, and anomalous current from Berry curvature associated with the Fermi surface. Importantly, by using the realistic band model for TaAs, we predicted that the SHG in TaAs is predominately contributed by the shift current, while the anomalous current has a minute contribution when the Weyl point is exactly located on the Fermi surface. Moreover, we highlight that the SHG contributed by the anomalous current decays fast with the increasing frequency of incident photons, and could be enhanced by proper electron or hole doping of TaAs. The anomalous Hall current is proportional to the inverse of photon energy of incident light. Topological semimetals have potential application for photodetector working in infrared to terahertz range. We also review recent experimental research on the nonlinear Hall effect of topological semimetal.

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S024

专题代号：S

Intrinsic magnetic topological insulators in van der Waals layered $MnBi_2Te_4$-family materials

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摘要：The interplay of magnetism and topology is a key research subject in condensed matter physics and material science, which offers great opportunities to explore emerging new physics, like the quantum anomalous Hall (QAH) effect, axion electrodynamics and Majorana fermions. However, these exotic physical effects have rarely been realized in experiment, due to the lacking of suitable working materials. In this talk, we will present our recent findings of intrinsic magnetic topological insulators in van der Waals layered $MnBi_2Te_4$-family materials [1-6]. The materials intrinsically show two-dimensional (2D) ferromagnetism in the single layer and three-dimensional (3D) *A*-type antiferromagnetism in the bulk, which could serve as a next-generation material platform for the state-of-art research. We predict extremely rich topological quantum effects with outstanding features in an experimentally available material $MnBi_2Te_4$, including a 3D antiferromagnetic topological insulator (AFM TI) with the long-sought topological axion states, the type-II magnetic Weyl semimetal (WSM) with one pair of Weyl points, and intrinsic QAH insulators and axion insulators. Experimentally, we confirmed the existence of 3D AFM TI phase [2], observed quantum phase transitions from axion insulator to Chern insulator [5], and further discovered high-Chern-number and high-temperature quantum Hall effect without Landau levels in $MnBi_2Te_4$ [6].

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S025

专题代号：S

Pseudospin and topological phenomena in Dirac-like photonic lattices

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摘要： Dirac materials such as graphene and topological semimetals have attracted enormous interest in condensed matter physics. The low energy electrons in Dirac materials behave as massless relativistic particles and obey the massless Dirac- Weyl equations which give rise to many exotic phenomena. Recently, the quasi- relativistic physics has been extended to classical wave systems. In optics, Photonic lattice composed of evanescently coupled waveguide arrays provides a useful platform to study the Dirac physics and topological phenomena. As the paraxial wave equation (describing propagation of light through a waveguide array) is mathematically equivalent to the Schrödinger equation (describing time evolution of electrons), this enables the study of analogies with various quantum and topological phenomena in condensed matter systems, providing novel ways to control the flow of light in photonics. Furthermore, photonic lattices offer exquisite control over initial conditions and allow direct observation of the actual wavefunction (including phase), features that are virtually impossible in electronic systems. In this talk, I will present some of our recent work based on Dirac-like photonic structures, including valley vortex states and degeneracy lifting via photonic higher-band excitation[1], and unconventional flatband localized states protected by real-space topology[2]. I will then focus on discussing pseudospin-orbit angular momentum conversion and universal momentum-to-real-space mapping of topological singularities arising from the interplay of Berry phase, pseudospin, and orbital angular momentum of light [3].

关键词： Photonic lattice, Pseudospin states, Dirac cone, Flatband states

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S026

专题代号：S

Topological Quantum Chemistry and its applications in materials search

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摘要：Here we propose a complete electronic band theory, which builds on the conventional band theory of electrons, highlighting the link between the topology and local chemical bonding. For all 230 crystal symmetry groups, we classify the possible band structures that arise from local atomic orbitals, and show which are topologically non-trivial. Our electronic band theory sheds new light on known topological insulators, and can be used to predict many more. In addition, an open-source code -CheckTopologicalMat- is released at https://www.cryst.ehu.es/cryst/checktopologicalmat or https://github.com/zjwang11/irvsp, which can be used to check the topology of any material by yourself. Finally, we perform a high-throughput search of 'high-quality' materials (for which the atomic positions and structure have been measured very accurately) in the Inorganic Crystal Structure Database in order to identify new topological phases. Among them, we present some topological materials to demonstrate the new topology in crystals.

关键词：拓扑量子化学，拓扑绝缘体，拓扑电子态

S027

专题代号：S

石墨烯拓扑界面态的研究

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摘要：石墨烯拓扑界面态具有独特的拓扑性质和输运性质。随着其在石墨烯体系和人工石墨烯体系的一系列重要实验进展，它们成为了拓扑态研究的一大热点。本报告将介绍过去一年来在石墨烯拓扑界面态方面的研究。我们发现石墨烯两种常见拓扑界面态的关系，并利用它们构建了有带隙的拓扑界面态和拓扑角态，进一步我们在石墨烯光子晶体观察到了这两种拓扑态，并讨论了它们的可能用途。我们研究了在半导体二维电子气构造人工石墨烯拓扑界面态，并以此为基础设计马约拉纳费米子理论方案。相比于纳米线一维拓扑超导，该方案有可调性强、对无序鲁棒、与半导体工艺兼容等特点，在实际应用中有较多的优势。

关键词：拓扑界面态、拓扑corner态、马约拉纳费米子

S028

专题代号：S

Weyl points and nodal rings in phononic semimetals

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摘要：Topological semimetals are materials whose band structure contains touching points that are topologically nontrivial and can host quasiparticle excitations that behave as Dirac or Weyl fermions. These so-called Weyl points not only exist in electronic systems, but can also be found in artificial periodic structures with classical waves, such as electromagnetic waves in photonic crystals and acoustic waves in phononic crystals. Due to the lack of spin and a difficulty in breaking time-reversal symmetry for sound, however, topological acoustic materials cannot be achieved in the same way as electronic or optical systems. And despite many theoretical predictions, experimentally realizing Weyl points in phononic crystals remains challenging. Here, we experimentally realize Weyl points in a chiral phononic crystal system, and demonstrate surface states associated with the Weyl points that are topological in nature, and can host modes that propagate only in one direction. As with their photonic counterparts, chiral phononic crystals bring topological physics to the macroscopic scale. Three-dimensional topological nodal lines, the touching curves of two bands in momentum space, which give rise to drumhead surface states, provide an opportunity to explore a variety of exotic phenomena. However, solid evidence for a flat drumhead surface state remains elusive. Here, we report a realization of three-dimensional nodal line dispersions and drumhead surface states in phononic crystal. Profiting from its macroscopic nature, the phononic crystal permits a flexible and accurate fabrication for materials with ring-like nodal lines and drumhead surface states. Phononic nodal rings of the lowest two bands and, more importantly, topological drumhead surface states are unambiguously demonstrated. Our system provides an ideal platform to explore the intriguing properties of acoustic waves endowed with extraordinary dispersions.

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S029

专题代号：S

高阶光子拓扑绝缘体

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摘要：近年来，对于拓扑物质相的研究已经从传统凝聚态领域扩展到光子系统，导致了一系列具有鲁棒性的光学器件的设计和实现，引起了人们的广泛的关注。作为一个典型的代表，传统的拓扑绝缘体具有鲁棒性的边界态传输，而其边界态是比系统的维度低一个维度。比如，一个三维拓扑绝缘体的受拓扑保护的表面态是二维的。近日，一种被称为高阶拓扑绝缘体的，具有更低维度边界态的新型拓扑绝缘体方案被提出。在三维情况下，其可能具有一维铰链态和零维拐角态。之前的方案都是基于需要在格点之间引入负耦合的拓扑多极子绝缘体。然而在光学系统中，引入格点之间的负耦合并不容易，需要复杂的结构设计。因此，我们在国际上首次提出利用二维全介质光子晶体，亦可以实现二阶拓扑绝缘体相和零维拐角态 [1]。我们在四方晶格的元胞内对称设置四个介电柱子，模拟四个人工原子。通过扩张和收缩这四个柱子的位置，实现了系统从拓扑平庸绝缘体相到非平庸绝缘体相的演变。通过数值模拟，发现在非平庸构型的四个拐角处，存在四重简并的局域态，即拓扑拐角态。其频率在带隙中为6.26GHz. 利用微波光子晶体系统和近场扫描技术，我们实验上证实了理论预言 [2]。为了刻画高阶拓扑相，我们基于拓扑晶体绝缘体理论，利用动量空间高对称点的旋转算符本征值，定义了一种新型拓扑拐角指标。其能够更精确的刻画出拐角态具有分数光子本征态的特征。本方案同时具有一维边界态和零维拐角态，显示出一种高阶拓扑相关于空间维度的层级现象。

关键词：高阶拓扑绝缘体；拓扑晶体绝缘体；全介质光子晶体；拐角态

S030

专题代号：S

铁磁拓扑材料的理论设计

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摘要：近年来，拓扑材料（拓扑绝缘体、拓扑半金属等）作为一种全新的量子态引起了物理学家和材料学家们的广泛关注。拓扑材料中零耗散的拓扑边缘态或表面态在未来的电子技术发展和信息领域中有着巨大的应用潜力，寻找和设计具有化学稳定性和环境友好的理想拓扑材料成为目前人们关注的焦点。最近，基于对称性指标法的非磁拓扑材料的理论设计研究取得了巨大的成功。相对于非磁性的拓扑材料，铁磁拓扑材料由于其磁基态的复杂性和磁空间群的多样性，研究相对缓慢。重要的是，铁磁拓扑材料中共存的本征磁化和非平庸电子态将具有广阔的自旋电子学应用前景。在我们工作中，根据第一性原理计算和对称性分析，在磁性拓扑绝缘体和拓扑半金属方面开展了相关工作。本报告主要介绍具有偶数对外尔点的铁磁外尔半金属、以及相对于自旋轨道耦合能稳定存在的结线半金属、三维量子反常 Hall 绝缘体等。

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S031

专题代号：S

Optimization of the intrinsic magnetic topological insulator $MnBi_2Te_4$ and transport study

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摘要：Quantum magnetic topological states combining the topological anomaly and magnetic order, such as quantum anomalous Hall (QAH) states and topological axion insulating states, emerge rich exotic quasiparticles with or without counterparts to mimic real particles in universe, of which further in-deep studies and potential applications, such as the prestigious quantum device, are extremely limited by the lack of suitable intrinsic magnetic topological insulators (MTIs). Here, we grow single crystals of the $Mn(Sb,Bi)_2Te_4$ family as part of a search for intrinsic MTIs, and by combining the angle-resolved photoemission spectroscopy, low-temperature transport, and first-principles calculations, we investigate the band structure, transport properties, and magnetism, as well as the evolution of topological anomaly in this family of materials. Taking careful consideration of the multiple transition processes of charge carriers, magnetization, and topology, we conclude that there exists an ideal MTI zone in the $Mn(Sb,Bi)_2Te_4$ phase diagram, hosting a potential high-temperature QAH effect, as well as possible for device applications. We also report the reserved anomalous Hall effect (AHE) in the $MnBi_2Te_4$ thin film. By employing the top/bottom gate, a negative AHE loop gradually decreases to zero and changes to a reversed sign. The reversed AHE exhibits distinct coercive fields and temperature dependence from the previous AHE. It reaches the maximum inside the gap of the Dirac cone. The reversed AHE is attributed to the competition of the intrinsic Berry curvature and the Dirac-gap enhanced extrinsic skew scattering. Its gate-controlled switching contributes a scheme for the topological spin field-effect transistors.

关键词： magnetic topological insulator; anomalous Hall effect

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S032

专题代号：S

Chiral broadband terahertz wave emission from the Weyl semimetals

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摘要：As a fascinating topological phase of matter, Weyl semimetals host chiral fermions with distinct chiralities and spin textures. Optical excitations involving those chiral fermions can induce exotic carrier responses, and in turn lead to novel optical phenomena. Here, we discover strong coherent chiral terahertz emission from the Weyl semimetals and demonstrate unprecedented manipulation over its polarization on a femtosecond timescale. Such polarization control is achieved via the colossal ultrafast photocurrents arising from the circular or linear photogalvanic effect. We unravel that the chiral ultrafast photocurrents are attributed to the large band velocity changes when the Weyl fermions are excited from the Weyl bands to the high-lying bands. The photocurrent generation is maximized at near-IR frequency range close to 1.5 eV for TaAs. Our findings provide an entirely new design concept for creating chiral photon sources using quantum materials and open up new opportunities for developing ultrafast opto-electronics using Weyl physics.

关键词： Weyl semimetal; Terahertz; Ultrafast photocurrent; circular photogalvanic effect

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S033

专题代号：S

Topological Understanding on the Lithium Storage Properties at the Interfaces of Transition Metal Oxide Hybrids

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摘要：The Li-ion storage properties of transition metal oxides (TMOs) are usually enhanced by different strategies, ranging from nanostructuring to hybridization and structural modification, which means that enriching these TMO electrode materials with definite functions is of great influence but highly challenging towards achieving high performance. [1] As a proof of concept, considering some common TMOs, several attempts have been employed to demonstrate the large variations in lithium storage performance of these TMOs, [2] but topological understanding on the adsorption capability at the electrode and current collector interfaces is rarely reported. Herein, the Li-ion storage chemistry of these TMOs is successfully deciphered by modulating the position of the p-orbital energy level via morphological engineering. Experimental analyses reveal that performance enhancement is related to the strong electronic modulations at the interface of the TMOs and the current collectors. [3, 4] Theoretical calculations predict that the modified TMO hybrids displayed reasonable lower adsorption energy towards easier Li-ion intercalation. [3, 4]According to density of states, such electronic modulations allow the shift of the p-adsorption energy towards accommodating interfacial electron transfer and facilitating rapid kinetics that helps in promoting the Li storage activity. [4]

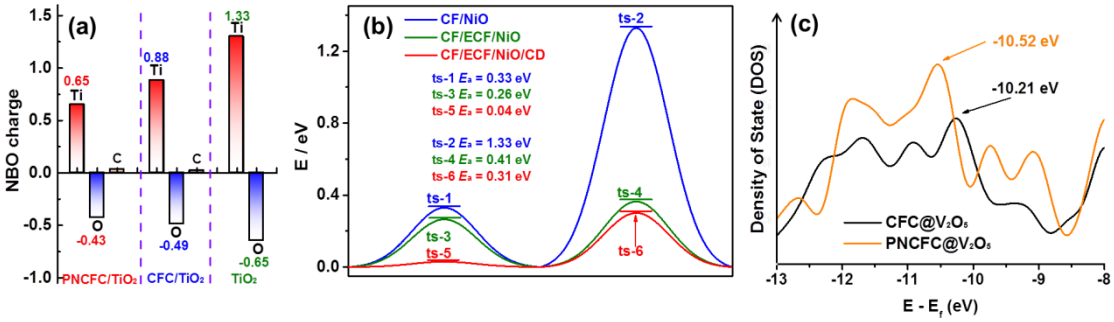

Figure 1 (a) NBO charge redistribution of TiO_2 hybrids. (b) Gibb's free adsorption energy (△G) profile of Li-ion intercalation via NiO hybrids. (c) DOS plots of V_2O_5 hybrids and their corresponding p-bands.

Keywords: transition metal oxide, Li-ion storage chemistry, DFT calculations, adsorption energy

Acknowledgement

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S034

专题代号：S

在合成空间中探索拓扑光子效应

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摘要：我们研究了一个环型微纳谐振腔系统，其介电常数被动态调制。在这个系统中，我们提出了一个合成空间概念，包含了光的频率维度。在这个系统中，每一个环型谐振腔支持一系列谐振模式，而我们假设这些谐振模式之间的频率间隔是近似一致的。我们选择了合适的动态调制模式，有效地连接这些谐振模式进而得以生成一个合成频率维度。在此基础之上，加入空间维度，我们就得到了一个高维的合成空间。在这个合成空间中，每个环型谐振腔上的调制相位能够被用来产生一个作用于光子上的等效磁场，并打破系统的时间反演对称性。我们利用该有效磁场来研究合成空间中的拓扑光子学问题，实现受拓扑保护的单向表面态。该表面态不仅在空间上有单向传输特性，而且在合成频率维度，该表面态也有单向传播性质，从而使人们能够有效的转换光的频率。这一系列的研究为现代光子学提供了一个新颖的平台，使我们能够在一个低维的物理结构中研究一个高维度的拓扑光子学问题。此外，在该合成空间中实现拓扑光子学特性，也为人们在空间以及频率维度上操控光子提供了多种可能性。

关键词：微纳谐振腔；动态调制；合成频率维度；拓扑光子学

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S035

专题代号：S

Quantitative analysis of weak antilocalization effect of topological surface states in topological insulator $BiSbTeSe_2$

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摘要：In topological insulators, the electrons' spin in topological surface states (TSS) is locked to its momentum, which gives rise to a non-trivial Berry phase after completing a time-reversed self-intersecting path adiabatically in the quantum diffusion regime.[1,2] This non-trivial Berry phase could lead to quantum correction to the classical electronic conductivity in low magnetic fields, manifesting itself as a weak antilocalization (WAL) effect.[3-5] Quantitative analysis of the WAL effect of TSS in topological insulators is of tremendous importance as it provides a strategic way to insight into the topological properties of the TSS. The major obstacle to achieve accurate results is how to eliminate the contribution of the anisotropic magnetoconductance of bulk states when the Fermi level lies in bulk bands.

Here, we demonstrate an alternative approach for the quantitative analysis of the WAL effect of TSS in a more accurate way by measuring anisotropic magnetoconductance of topological insulator BiSbTeSe2 (BSTS). The anomalous conductance peaks in the parallel orientations are observed in anisotropic magnetoconductance curves, which are originated from the WAL effect of TSS of BSTS. By subtracting the anisotropic magnetoconductance of bulk states, the WAL effect of topological surface states can be well described by the Hikami-Larkin-Nagaoka expression. Our findings offer an alternative avenue for the quantitative exploration of the WAL effect of TSS in topological insulators.

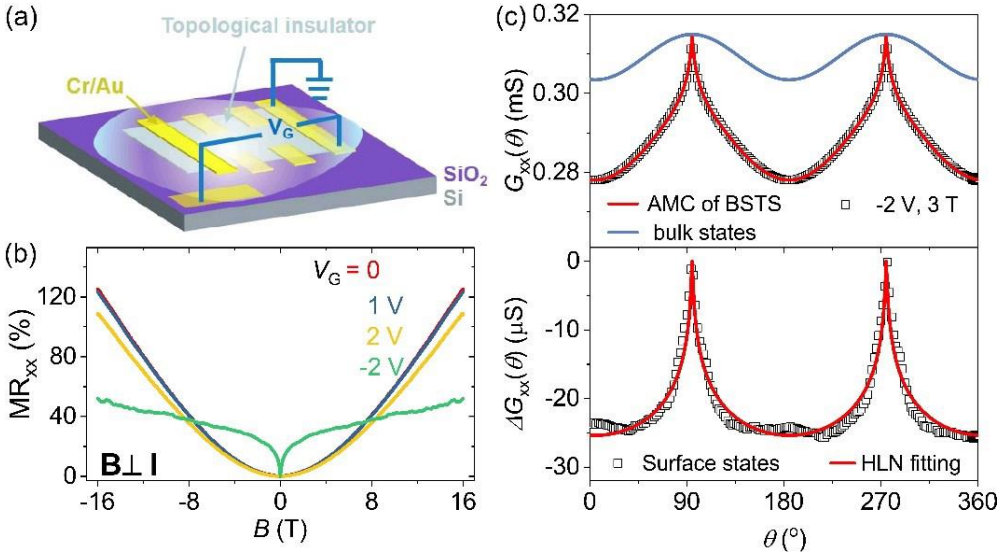

Fig.1. (a) Schematic drawing of the BSTS device. (b) Magnetoresistance (MR) curves of BSTS devices at low B-

fields and at different gate voltages and 2 K. (c) (top) Angular dependence of the longitudinal sheet conductance Gxx for VG = -2 V. The red solid line is the fitting curve. The blue solid line is the fitting curve of the anisotropic magnetoconductance of bulk states. (bottom) Angular dependence of the Gxx, which is the difference between Gxx(θ) and the blue curve in the top panel. The red solid line is the fitting curve using HLN expression.

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S036

专题代号：S

Visualization of topological kink states and corner states in two dimensional photonic crystals

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摘要：Topology physics is bringing new development to optics. Unidirectional optical waveguides without external magnetic field will be essential to optical communications. An optical analogy to quantum spin Hall effect is visualized using deformed honeycomb lattices of dielectrics [1], which can be straightforwardly extended optical frequencies. Photonic valley kink states in photonic crystals are exploited and future optical devices such as valley filter and valley coupler are proposed [2].

Domain walls with kink states can be created by engineering a honeycomb lattice structure, where quantum spin Hall effect is possible by lattice deformation and valley kink states are induced by sublattice symmetry breaking. We find that the coexistence of these two mechanisms gives rise to topological corner states [3] and various applications to graphene can thus be studied. The common topology principle shared by condensed matter systems and photonic crystals makes photonic system a perfect platform to visualize the corresponding physics, because of its convenient sample preparation and measurement. Moreover, by introducing novel concepts in topology physics to photonic crystals, novel design principles to optical devices can be thus motivated.

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S-P001

专题代号：S

基于表面离子栅调控技术下的氧化锌纳米线材料的气敏性能研究

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摘要：如今社会发展日新月异，纳米科技的实现为氧化物气敏传感器性能的进一步提高带来了巨大助力，但氧化物气体传感器还存在工作温度过高这一突出问题，会引起使器件出现结构复杂性增大，能耗过高等消极影响，脱离物联网的快速发展背景下人们对气体传感器提出的微型自驱动化的要求，为此，降低气体传感器的工作温度，是本篇工作的主要研究内容。

摩擦纳米发电机（TENG）自2012年被提出后，在能源收集，自驱动传感等领域受到广泛的关注。TENG由于具有输出电压高、输出电流小的特点，容易电离空气。我们课题组利用TENG在空气条件下实现了气体放电，并通过摩擦纳米发电机对O_2、CO_2等不同分子进行电离，研究了活性负离子的产生过程和机制。本文使用我组提出的基于摩擦纳米发电机气体离子栅调控技术，使O_2先电离成O_2^-，然后再吸附在氧化物的表面，利用该技术有望可以提高O_2^-的吸附数量与吸附速度，解除氧化物气敏传感器的高温工作条件这一技术壁垒，成为实现气敏传感器室温传感的一个全新的技术手段。

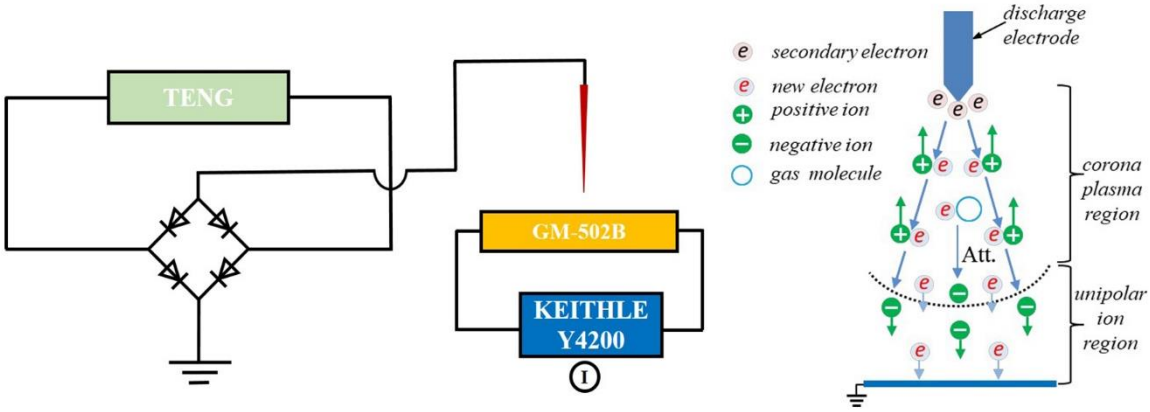

图1 表面离子栅调控原理及负电晕放电离子运动示意图

关键词： 氧化锌，摩擦纳米发电机，表面离子栅调控，气敏性能

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S-P002

专题代号：S

脉冲激光沉积制备$Sb_2Te_3/Bi_2Te_3/Sb_2Te_3$量子阱的热电性能研究

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摘要：随着全球经济的发展，能源和环境问题变得日益严峻，因此寻找高效又环保的能源转换技术成为当今世界各国科学工作者的研究重点。热电材料制成的热电器件具有结构简单、体积小，重量轻；工作时绿色环保、超静音、零磨损；无运动部件、使用寿命长等优点。热电材料能够在能源领域的大规模应用，不仅需要提高材料的热电优值（ZT），也离不开成熟的产业化制备方法。掺杂和材料低维化是目前降低晶格热导率的最主要途径。1993年hicks等[15,16]提出了材料的低维化以及超晶格量子阱等特殊的结构能提高材料热电性能的预测及理论计算，认为当材料从三维（3D）晶体过渡到低维材料时，量子阱（2D）、量子线（1D）及量子点（0D）的热电性能远远超过块体材料。在这里，我们采用脉冲激光沉积（Pulsed Laser Deposition）技术在室温下的p型Sb_2Te_3衬底上生长n型Bi_2Te_3和p型Sb_2Te_3薄膜，并对制备的薄膜进行XRD和SEM表征，得到薄膜的化学计量组成以及结构，制备得到具有高热电性能的量子阱结构，以这种量子阱结构为基础制成的薄膜热电器件，具有较小的尺寸与半导体处理技术的兼容性，其在微电子器件等领域有较大的应用前景。

关键词：热电 低维 薄膜 量子阱

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S-P003

专题代号：S

拓扑光子晶体陈数的数值计算

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摘要：拓扑光子晶体是拓扑绝缘体在光学系统中的类比，具有包括存在拓扑保护的手性边界态在内的诸多良好性质，在光信号调制、微腔应用等方面具有广泛的应用前景。然而，人工优化拓扑结构效率较低，参数空间利用不充分，费时费力。而随着电子计算机性能的提升、数值方法以及智能优化算法的发展，基于智能算法的拓扑结构优化能够减少人工成本，打破传统结构限制，为拓扑结构的优化设计提供新思路。为此，需要寻找普适的拓扑态判据与数值计算方法。对于二维拓扑光子晶体，陈数是一个重要的拓扑标志量。因而，陈数的数值计算对于实现拓扑结构的算法优化具有十分重要的意义。本文作者在T. Fukui等人的工作的基础上，基于有限元软件COMSOL Multiphysics设计了一套普适的光子晶体Berry曲率以及陈数的数值算法。在此工作中，分别计算了几种典型的旋磁光子晶体结构与谷光子晶体结构Berry曲率分布与陈数。对于旋磁光子晶体，陈数可以很好地标志其拓扑性质；对于谷光子晶体，由于时间反演对称性保护，其陈数为0，但其拓扑性质可以通过高对称点K/K'附近Berry曲率的符号判断。随后，通过计算几种拓扑结构的边界模式，验证了拓扑边界态的存在。该方法可以实现目前所有典型的二维拓扑光子晶体的陈数和Berry曲率分布的计算，对拓扑光子晶体的算法实现具有重要意义。

关键词：拓扑光子晶体 陈数 数值计算

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S-P004

专题代号：S

Giant anomalous Nernst effect in the magnetic Weyl semimetal $Co_3Sn_2S_2$

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摘要内容:　在金属铁磁材料中，Weyl 点附近的 Berry 曲率引起垂直于磁化和电流方向的电压，这种不需外磁场参与产生横向电压的现象，称为反常 Hall 效应。与反常 Hall 效应对应的热电效应，称为反常 Nernst 效应。我们对铁磁 Weyl 半金属 $Co_3Sn_2S_2$ 进行了 Nernst 测量，在 Curie 温度下得到的最大反常 Nernst 信号 Syx ~ 5μV/K。比先前报道的 Mn_3Sn 等铁磁体的最大值还要大一个量级。此外，我们实验得到的反常横向热导系数在 70K 时高达 10A/K，在已知的半金属材料中是最大的，提供了一个强有力的证据证明反常 Nernst 效应也是费米能级附近手性 Weyl 点的 Berry 曲率引起的。

关键词: $Co_3Sn_2S_2$， Weyl semimetal，ferromagnetic，giant anomalous Nernst effect

S-P005

专题代号：S

应力状态下碲化汞中多种拓扑相的非线性霍尔效应

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摘要：在传统的霍尔效应中，纵向电流和横向电压呈线性关系，并且体系的时间反演对称性需要被破坏。最近，傅亮等人首先在具有时间反演对称性的体系中预言了一种二阶非线性霍尔效应。这一效应是指在体系中通特定方向的低频振荡电流时会在某些方向产生一个直流和倍频的二阶响应电流。这种效应起源于贝利曲率偶极子，即贝利曲率的一阶矩。不为零的贝利曲率偶极子要求体系必须破坏空间反演对称性，从而对体系的对称性提出了限制。值得一提的是，这一效应很快在最近的几个实验中得到证实，并引起了广泛的研究兴趣。然而，之前的研究主要集中于二维拓扑体系，对于三维拓扑体系的研究还很少。

三维碲化汞体系满足非线性霍尔的对称性要求，并且我们之前的工作预言在不同应力状态下体系可以实现多种拓扑相，包括理想外尔半金属相、节线半金属相、第二类外尔半金属相及拓扑绝缘体相。因此，仅仅调节应力就可以得到丰富的拓扑相以及相应的非线性霍尔效应。基于$\mathbf{k}\cdot\mathbf{p}$模型，我们计算了不同拓扑相的贝利曲率偶极子随费米能调节变化的曲线，以探索不同拓扑相之间非线性霍尔效应的区别和联系，这或许会为区分拓扑相提供一个不同的实验观测角度。

关键词：非线性霍尔效应 贝利曲率偶极子 $\mathbf{k}\cdot\mathbf{p}$模型 碲化汞 拓扑相

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S-P006

专题代号：S

The Novel Thermal Spin Transport Properties based on Low-dimensional Nanoscale Materials

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摘要： s a new subject, spin caloritronics has been a hot topic of various research fields in recent decades. Different from traditional spintronics, it deals with the interactions of heat, spin and charge currents induced by the temperature gradient. The research includes two aspects: on the one hand, exploring the new mechanism of generating the spin-Seebeck effect; on the other hand, looking for new functional magnetic materials having a good symmetrical spin current together with high spin figure of merit. We use the density functional theory calculate the band structures and spin density, and the nonequilibrium Green's function method analysis the thermal spin transport properties. The main findings are as follows in details: (i) Based on four homojunctions systerms, the thermal spin current is explored and our researches reveal a ferromagnetic metallic γ-graphyne exhibits transport properties similar to those of the ferromagnetic semiconductor. Here, we proposed a new mechanism called the compensation effect originating from the concellation of electrons and holes around the Fermi level to produce a net spin-up or spin-down transport channel; (ii) To explore reliable material platforms and uncover new rules to realize spin-Seebeck effect (SSE) and thermal spin-filtering effect (SFE), we construct several magnetic BNNTs. We find that a high rotational symmetry of the carbons contributes to generate the SSE with more symmetric thermal spin-up and spin-down currents, otherwise towards the thermal SFE. More importantly, we find that the compression strain engineering is an effective route to improve these effects and to realize the transition between them; (iii) To realize a good spin-Seebeck effect (SSE) together with high spin thermoelectric conversion efficiency (TCE), two nanoscale structures referred to as nanoribbons and nanotubes have been studied systematically and comparatively. Our theoretical results show that although these two different structures display similar spin semiconducting states, the BNNRs have lower lattice thermal conductance due to the phonon scattering at edges, contributing to the enhancement of the spin figure of merit; while the BNNTs can generate a better SSE and larger spin thermopower, due to the rotational symmetry.

S-P007

专题代号：S

Dynamic properties of terahertz quantum cascade lasers under optical injection

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摘要:　我们对自由运行，主从注入，互注入的 THz QCLs 进行了理论研究。 我们比较了三种这三种情况下的自发辐射噪声和调制响应特性。 特别是，对于相互注入的 THz QCL，我们在不同的工作条件下详细计算了电场和功率谱。 这些结果有助于进一步了解光注入时 THz QCLs 的非线性动力学行为。我们展示了 THz QCL 互注入阵列用于速度传感的模拟结果。这些理论研究为 THz QCL 锁相阵列及相关应用的发展提供理论支持。

关键词: 太赫兹，量子级联激光器，光注入，速度测量

S-P008

专题代号：S

Pressure-tuned colossal magnetoresistance effect in *n*-type $CdCr_2Se_4$

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摘要: Colossal magnetoresistance (CMR) effect in Cr-based spinels ACr_2X_4 (A = Cd, Hg; X = S, Se) has potential applications in magnetic devices. Numerous publications about element substitution or chemical doping in the spinels have been reported in order to optimize the CMR effect through tuning the type of carrier, carrier density or lattice structure. Since high pressure has been a fruitful route for tuning lattice as well as electronic states, we have performed high pressure measurements on *n*-type $CdCr_2Se_4$ to investigate the evolution of colossal magnetoresistance effect with increasing pressure. The high-pressure electrical transport and magnetization measurements show that the colossal magnetoresistance effect is suppressed continuously upon compression, accompanied with the decline of ferromagnetism. The present findings prove the tight connection between electrical transport, magnetism and structure in the *n*-type $CdCr_2Se_4$, which provides one effective path to tune the colossal magnetoresistance effect by pressure.

关键词：CMR　*n*-type $CdCr_2Se_4$　high pressure

S-P009

专题代号：S

拓扑材料的单晶生长和物性研究

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摘要：近期，对于拓扑材料的研究特别的活跃，自从第一个拓扑绝缘体发现以来，拓扑的概念深入到凝聚态物理学的各个领域,极大地推动了现代物理学的发展，拓扑光子学,拓扑半金属,拓扑超导体以及磁性拓扑材料各个研究方向齐头并进。此外，具有与材料表面结构无关的内禀物理特性和稳定的拓扑保护性质，也有可能在未来的电子技术发展和信息领域中获得众多应用，有着极大的应用潜力。

人们常用的单晶生长方法包括高温溶液方法，化学气相输运，助熔剂法，水热法，Bridgman法等，我们主要通过助溶剂法和化学气相输运等方法，生长了高质量的拓扑材料晶体，其中包括$MnBi_2Te_4$、$EuIn_2As_2$ 、$EuIn_2P_2$等磁性拓扑材料，Srx Bi_2-xSe_3等拓扑超导材料，(TaSe4)2I等weyl半金属，以及其他热门单晶拓扑材料，并且通过EDS、XRD等手段对其进行了表征。另外，我们对$(TaSe_4)_2I$ 、$MnBi_2Te_4$和Srx Bi_2+xSe_3等进行了电学测试，对$EuIn_2As_2$ 、$EuIn_2P_2$等磁学和电学方面的研究，取得了一些进展。同时，我们与国内外其他许多实验课题组进行密切合作，包括STM，ARPES，光电，高压等测试研究，并取得了一些进展。

S-P010

专题代号：S

新型拓扑超导体预测：beta-RhPb2

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摘要：我们通过第一性原理方法预测了一种新的拓扑超导体：beta-RhPb2。该材料拥有非平庸的拓扑性质并且其涡旋型表面态恰好穿过费米面。通过电声耦合计算预测的超导转变温度高达9.7K。这意味着其体的超导电性可以通过超导近邻效应在表面态上打开超导能隙，实现拓扑超导电性。

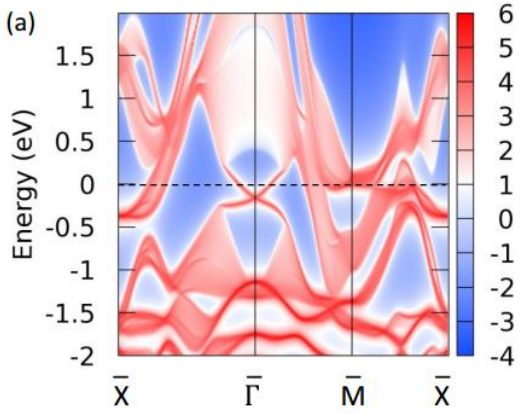

图1 beta-RhPb2恰好穿过费米能级的拓扑表面态

关键词：拓扑超导体 拓扑绝缘体 电声超导

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S-P011

专题代号：S

de Haas-van Alphen oscillation in topological semimetal $BaGa_4$

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摘要：We report the magneto-transport properties of $BaGa_4$ single crystal with the space group I4/mmm at low temperature. $BaGa_4$ exhibits large magnetoresistance (MR) ~ 3000% at 2 K and 14 T which submits to $B^{1.65}$ field dependence. Evident de Haas-van Alphen (dHvA) quantum oscillation at low temperature and high magnetic field have been observed with B//c configuration, from the analysis of which the multiple frequencies, the small effective masses and nontrivial Berry phases are extracted. Firstly, the multi-band Lifshitz-Kosevich (LK) formula fitting is applied to extracted Berry phases and several are closed to π. To aid reliability, Landau level (LL) index fan diagram is employed to analyze the Berry phase which are consistent with results of multiband LK fittings. The first-principles calculations elucidate that $BaGa_4$ possesses a Dirac point along Σ_1-N line which opens a tiny gap in the presence of spin-orbit coupling (SOC). The Z_2 invariant of $BaGa_4$ equals 1, indicating its nontrivial topological properties.

关键词： quantum oscillations, large magnetoresistance, nontrivial Berry phase, electronic structure, first-principles calculation, topological semimetal

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中央高校基本科研基金中国人民大学项目 （No. 18XNLG14, No. 19XNLG18）

S-P012

专题代号：S

The variation of the orbital magnetization during the localization route for quantum anomalous Effect.

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摘要：Haldane model is an important part of research of topological insulators. We study the influence of the disorder strength creating on the orbital magnetization of the Haldane model whether the Chern number of the topological insulator is nontrivial or not under clean condition. It's observed that in the nonzero Chen number case, the orbital magnetization displays a sharp increase before the Hall conductance collapse. When the disorder strength is large enough to destroy the quantum Hall platform and further cause Anderson localization, the orbital magnetization decreases from its maximum to zero following the Chern number from 1 to 0. This relation can be verified in the zero Chern number case, the biggest difference from the nonzero Chern number is that the orbital magnetization changes weakly within the finite small disorder strength. As the disorder strength increases to a value which is sufficient to affect the Chern number, the orbital magnetization has a closely connection with the quantized Hall conductance. Namely, if the Chern number increases, the orbital magnetization increases. On the contrary, the orbital magnetization decreases with the Chern number.

关键词： orbital magnetization, Haldane model, disorder

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S-P013

专题代号：S

Extremely large magnetoresistance and Shubnikov-de Haas oscillations in DyBi

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摘要：We report the magnetotransport properties of DyBi, a semimetal with antiferromagnetic ground state. DyBi adopts a rocksalt type crystal structure with space group of Fm-3m at room temperature, which changes to tetragonal structure with space group of I4/mmm at 10.5 K. Meanwhile, at low temperature, the magnetic structure of DyBi changes from MnO-type AFM to HoP-type, then to ferromagnetic (FM) with the increasing field. Both the structure transition and magnetic transition in DyBi are invoked to explain the anomalous kinks observed in resistivity curves. DyBi exhibits extremely large magnetoresistance (XMR) and Shubnikov-de Haas (SdH) oscillations at low temperature and high magnetic field. The Berry phase extracted from SdH oscillations suggests that DyBi might be topologically nontrivial. From the analysis of nonlinear filed-dependent Hall resistivity, compensated electron and hole (n_e=n_h) with high mobility (~10^{19}) has been observed, which is demonstrated to be the origin of XMR in DyBi.

关 键 词：Shubnikov-de Haas oscillations, nontrivial Berry phase, extremely large magnetoresistance, structure transition, magnetic transition, compensated electron and hole, high mobility

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S-P014

专题代号：S

热导率降低一个数量级的纳米结构Zr/$HfTe_5$单晶

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摘要：热电材料是一种能够直接将热能转化为电能的材料，且具有环境友好的特点，可用于发电机和无氟冰箱等领域，在材料和能源领域引起了广泛的关注。层状过渡金属五碲化物$ZrTe_5$和$HfTe_5$在室温下具有较高的电导率(>10^5 Ω^{-1} m^{-1})和塞贝克系数(> 100 μV/K)，因此有望成为良好的热电材料。但现有报道显示，$ZrTe_5$和$HfTe_5$的热导率较高，这对该材料的热电性能十分不利。为了降低$ZrTe_5$和$HfTe_5$晶体的热导率，我们通过优化生长参数，生长出具有纳米结构的$ZrTe_5$和$HfTe_5$单晶。晶体的生长机理是先成核然后成在晶核周围聚结成单晶。微观结构表征证实了纳米结构$ZrTe_5$和$HfTe_5$晶体具有长条状的镶嵌图案，条纹沿纵向具有纳米尺度的横截面和亚微米尺寸。为了进一步对比分析，我们还用助熔剂法得到了接近完美的$ZrTe_5$晶体。值得注意的是，纳米结构$ZrTe_5$和$HfTe_5$晶体的最大热导率可被抑制至0.45 W m^{-1} K^{-1}，比理论值低一个数量级，比接近完美的$ZrTe_5$和$HfTe_5$晶体的小三倍。热导率的计算分析，表明纳米结构$ZrTe_5$和$HfTe_5$晶体的声子平均自由程约为晶体单层厚度。同时拉曼光谱证实了纳米结构$ZrTe_5$和$HfTe_5$晶体中光学声子的准粒子寿命是声子输运寿命的近4倍，这从光谱的角度证明了微观结构对热导率的显著影响。我们的工作可以为通过控制晶体生长条件实现晶体微观结构调控来调节材料的导热系数提供一种有效的方法。

关键词：过渡金属五碲化物、晶体生长、热传输、拉曼光谱、纳米结构

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S-P015

专题代号：S

基于II类狄拉克半金属$PtTe_2$的太赫兹探测器

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摘要：太赫兹波段是介于红外和微波之间的频谱范围，太赫兹的频率从0.1THz到10THz，波长范围为0.03mm-3mm。众所周知，对于红外波段的研究推动了光子学的飞速发展与应用，对于微波波段的研究建立起来的无线电通信理论也已经得到了广泛的应用，介于这两者之间的太赫兹领域还处于研究阶段，其技术还远远落后于红外或者微波的水平，太赫兹也成为了电磁谱中唯一一块未被深入挖掘的领域。太赫兹波所具有的低能量、强穿透力等特点，在无损检测、安全检查和医学领域具有诱人的应用前景，由于其波段位于电子学科和光子学科的交叉领域，因此，对太赫兹光电探测的研究有助于两大前沿学科的融合发展。近年来，以石墨烯为代表的二维材料的光电性能得到快速发展，二维材料由于其独特的性质在太赫兹探测领域掀起研究热潮，许多材料如石墨烯[1]、黑磷等可用于制作场效应晶体管进行太赫兹的探测，二维材料作为晶体管的沟道提供二维电子气，载流子在源漏之间共振形成等离子体波，当共振频率接近太赫兹频率，等离子体将吸收太赫兹辐射在沟道内产生直流电压形式的光响应，实现对太赫兹的探测[2]。然而，石墨烯的零带隙意味着开关比的不足，因此，对高吸光度，高载流子迁移率材料的探索是光电子领域的挑战。$Bi_2Te_{3-x}Se_x$、$Bi_{2-x}Sb_xTe_3$等拓扑绝缘体作为新的拓扑量子态，它具有丰富的表面态能够与电磁场互相作用，在太赫兹探测等光电探测技术上展示出它的潜力[3]，因此，对拓扑绝缘体的研究有助于人们探索太赫兹探测的全新机理。本文报道了一种基于二维$PtTe_2$材料的高性能太赫兹光电探测器，器件结构如图所示。$PtTe_2$是一种新型的II类拓扑狄拉克半金属材料，相比较于I类狄拉克材料，它具有倾斜的狄拉克锥。基于它的表面态特点，我们设计出金属-$PtTe_2$-金属结构的太赫兹器件，利用太赫兹波与非平衡费米子的非对称耦合产生光电流，器件有效地对太赫兹波进行了探测，展现出优秀的探测器性能。二维材料具有的理想二维界面，层与层之间依靠范德瓦尔斯力结合，材料表面不存在悬挂键，因此，制备异质结结构将不受晶格常数和堆叠顺序的限制，同时异质结能结合不同材料的优点，构建范德尔瓦尔斯异质结可以实现新的功能光电器件[4]。基于此特点我们将$PtTe_2$与石墨烯结合形成异质结，$PtTe_2$和石墨烯之间强烈的内建电场加速了非平衡载流子的移动，提升了探测器的探测效率，因此验证了基于异质结构的太赫兹探测器是一个有效的探测手段。这些结果预示着$PtTe_2$等II类狄拉克半金属在太赫兹波段的探测上可作为理想的材料进行研究应用。

关键词：太赫兹探测，拓扑半金属，范德尔瓦尔斯异质结

S-P016

专题代号：S

基于新型拓扑绝缘体碲化银的宽波段光电探测器

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摘要：传统半导体光电探测器在特定波段内已有较好的工作表现，但由于其禁带限制，在宽波段、尤其远红外的光电探测中仍有一些困难。无带隙的拓扑材料是实现宽波段探测的一种理想选择，石墨烯是该方向的重点研究对象之一，然而单层石墨烯的光吸收率极低，多层结构又会失去其无带隙特性，因此很难投入实际应用。碲化银（β-Ag_2Te）是一种新型的三维拓扑绝缘体[1]，其表面态中存在高度各向异性的狄拉克锥结构，与此前研究较多的其他拓扑材料（如Bi_2Te_3, Bi_2Se_3等的狄拉克锥均为各向同性）具有很大的不同。一方面，碲化银很好地兼备了无带隙特性和较高的吸收率；另一方面，狄拉克锥的各向异性使其能够对不同的旋光偏振状态做出响应；此外，这种材料还具有超高的载流子迁移率。因此，碲化银在高效宽波段光电探测以及偏振探测中表现出较大的潜力。

我们通过化学气相沉积技术生长了高纯度、高质量的碲化银单晶纳米片，并采用一系列微纳加工工艺将其制作成光电探测器件。实验结果显示，碲化银在室温下已具有优秀的光电流响应特性，可见光到红外波段激光均能被有效探测，与此同时光电流表现出明显的偏振依赖性。

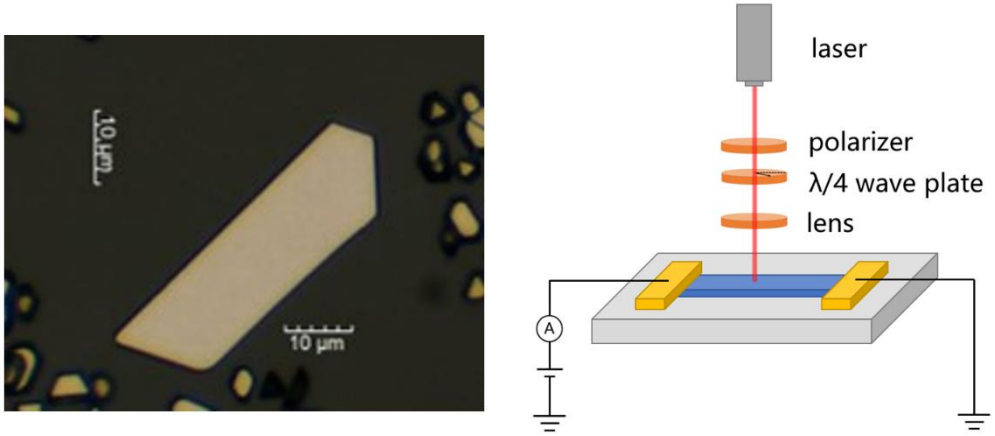

图1 化学气相沉积法制备的碲化银纳米片及光电探测示意图

关键词：碲化银 宽波段光电探测器 拓扑绝缘体

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S-P017

专题代号：S

Log-periodic Quantum Oscillations and Discrete Scale Invariance in Topological Materials

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摘要内容: Quantum oscillations are usually the manifestation of the underlying physical nature in condensed matter systems. Here, we report a new type of log-periodic quantum oscillations in ultraquantum three-dimensional topological materials. Beyond the quantum limit (QL), we observe the log-periodic oscillations on the magnetoresistance and the Hall traces of high-quality single-crystal ZrTe5 and HfTe5, virtually showing the clearest feature of discrete scale invariance (DSI). Further, theoretical analyses show that the two-body quasi-bound states can be responsible for the DSI feature. Our work provides a new perspective on the ground state of topological materials and Dirac materials and evidences the universality of the DSI in the Dirac materials.

关键词: log-periodic oscillations, discrete scale invariance, topological materials, Dirac materials, magnetoresistance, Hall resistance

S-P018

专题代号：S

Single crystal growth and magnetoresistivity study of topological semimetal $SrAs_3$ on micro fabricated devices

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Abstract: The study of topological semimetals has attracted huge interest from both the theoretical and the experimental communities in recent years. For topological nodal line semimetals, the band crossing points form loops instead of discrete points. Topological nodal line semimetals have many interesting expected properties, such as drumhead-like nearly flat surface states, unique Landau energy spectra. By first-principles calculations and a $k \cdot p$ model Hamiltonian analysis, $SrAs_3$ has been predicted to be a candidate for topological nodal line semimetals [1].

Our High-quality $SrAs_3$ single crystals are grown via the Bi flux technique. $SrAs_3$ has the monoclinic crystal structure with a low crystalline symmetry, which makes transport measurement difficult, as the current distribution in bulk sample is complicated. Focused ion beam(FIB) is a simple approach for fabrication of microstructures from crystalline material for electric measurements. By employing FIB, we have precise control over the crystal shape and get a v-shaped structure of $SrAs_3$ featuring two resistance bars, along well-defined crystal directions. Detailed measurements were carried out on the FIB fabricated single crystal transport devices. By Analysis of magnetoresistance, Shubnikov-de Hass (SdH) oscillations and Hall resistivity, we determine the electronic band structure and discuss possible topological properties of $SrAs_3$.

Key words: topological nodal-line semimetal, focused ion beam, microfabrication

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S-P019

专题代号：S

Torque Magnetometry Based on a Commercial Membrane-Type Surface Stress Sensor

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Abstract: High-quality single crystals are essential for the research of intrinsic magnetic properties. However the preparation of sizable samples for measurements is not always straightforward. Therefore, sensitive magnetometers are necessary. Torquemeters have proven to be a powerful tool for measuring magnetic moments, especially at high fields. Among the torquemeters, self-sensitive microcantilevers have a high force sensitivity and enable us to measure hundreds of micrometer sized samples. Rightnow, the number of commercially available self-sensitive microcantilever suitable for toqrue measurements is considerably limited, which gives us the motivation to search for alternatives.

In this work, new torquemeter based on commercially available membrane-type surface stress sensor (MSS) are adopted for the measurements of tungsten carbide (WC), which is demonstrated to be a topological semimetal with triply degenerate node. Clear de Hass-van Alphen oscillation signal is observed on single crystals with largest dimension about 300 micrometer. By fast fourier transform (FFT) analysis of the oscillation frequency, new frequencies were observed besides the ones reported in previous work[1], which indicates that the MSS is a good candidate for low temeterature, high magnetic field torque measurements.

Key words: torque magnetometry, membrane-type surface stress sensor, de Haas–van Alphen oscillation

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S-P020

专题代号：S

Coexistence of Quantum Anomalous Hall and Anomalous Valley Hall Effects in Metal-Organic Frameworks

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Abstract: Metal-organic frameworks (MOFs) are emerging as a new type of two-dimensional (2D) materials, which may own interesting topological behaviors. We here design a plane layered MOF $C_6H_3N_3Au$ which possesses C_{3v} symmetry, broken inversion symmetry, and spontaneous magnetism induced by the N atoms in the MOF. Using first-principles calculations, we find coexistence of quantum anomalous Hall (QAH) and anomalous valley Hall (AVH) effects in the system, happening exactly around the Fermi level. The two Hall effects are induced primarily by the C_{3v} symmetry protected two-fold degenerate N p_x/p_y orbitals hybridizing with certain Au $d_{xy}/d_{x^2-y^2}$ orbitals and the p_z orbitals from N and C atoms, respectively. How the strain and the strength of the spin-orbit coupling tune this unique multiple Hall effect coexistence phase is also explored. Our work may inspire more novel transport properties in future electronics, valleytronics, and spintronics.

Key words: Quantum anomalous Hall effect; Anomalous valley Hall effect; Topological state; First-principles calculation; Metal-organic framework

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S-P021

专题代号：S

基于三维狄拉克半金属砷化镉的宽波段光电探测器

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摘要：狄拉克半金属是一种全新的拓扑量子材料，有着诸多奇特的性质，如在狄拉克点处有线性色散的能带结构。这些不同寻常的性质使得狄拉克半金属在高性能光电探测器方面有着巨大的潜力。一个典型的例子是二维的狄拉克半金属—石墨烯。基于其线性色散能带、高载流子迁移率和零带隙等特点，石墨烯光电探测器件具有超快响应、宽波段探测等优点。而砷化镉材料，作为三维石墨烯，能够与光有更强的相互作用，从而达到更高的响应率。

本工作通过分子束外延生长技术在氧化铝衬底上获得了高质量的砷化镉薄膜，在此基础上制备了砷化镉薄膜探测器，实现了从可见光到红外范围的宽波段光电探测，并获得了较好的响应率。

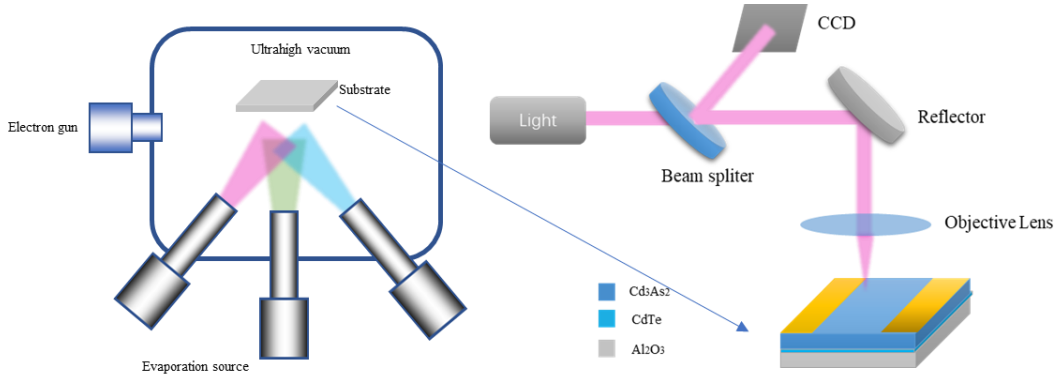

图1 砷化镉探测器件制备及光电探测示意图

关键词：砷化镉 三维狄拉克半金属 宽波段探测

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S-P022

专题代号：S

Quantum anomalous Hall insulators with high Chern numbers in antimonene monolayer

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Abstract: In this talk, we will mainly introduce the electronic and topological properties in square/octagon antimonene (so-Sb) monolayer doped with transition metal (TM) adatoms based on density-functional theory and effective model analysis. Interestingly, the quantum anomalous Hall state with a high Chern number C=4 for Mo doped so-Sb monolayer under a compressive biaxial strain (~ 5%) is predicted, as can be verified by four gapless chiral edge states inside the gap, extremely different from familiar Chern numbers (*i.e.*, C=±1 or ±2) obtained in TM doped honeycomb systems. The nontrivial bulk topology originates primarily from the band inversion of non-degenerate Mo $d_{x^2-y^2}$ and d_{xy} orbitals in the special tetragonal crystal field, which appears around the high symmetry M point in the Brillouin zone. The theoretical model calculations indicate that the topological state is determined by the adatom magnetism, crystal field from so-Sb and spin-orbit coupling. Our results demonstrate that the Chern insulating phase with a high Chern number C=4 will provide enhanced anomalous Hall conductivities to improve the transport capability for future antimonene-based spintronic devices.

S-P023

专题代号：S

Quantum magnetism of topologically-designed graphene nanoribbons

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摘要：Graphene nanoribbon (GNR) is a planer strip of graphene with extraordinary electronic and physical properties. It is first introduced as a theoretical model to study the size effect in graphene. Recent advance in bottom-up techniques have allowed production of atomically precise GNRs with armchair, zigzag and other sophistated edges. GNRs have potential applications in the next-generation nanoelectronics, and have been extensively investigated.

Based on the Hubbard models, quantum magnetism of topologically-designed graphene nanoribbons (GNRs) is studied using exact numerical simulations. We first study a two-band Hubbard model describing the low-energy topological bands. It is found the spin correlations decay quickly with the distance, and the local moment is extrapolated to zero in the presence of symmetry-breaking terms. We then include the Hubbard interaction to the topological-designed GNRs. For large interactions, the spin correlations keep finite for all distances, and the magnetic order develops. The local moment is extrapolated to almost zero for weak interactions, and begins to increase rapidly from a critical interaction. The estimated critical value is much larger than the realistic value in graphene, and we conclude the experimentally relevant GNRs is nonmagnetic, which is consistent with the experimental results.

关键词：graphene nanoribbon, density matrix renormalization group (DMRG), determinant quantum Monte Carlo (DQMC) simulation, mean-field (MF)

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S-P024

专题代号：S

磁近邻效应诱导下β硼烯中完全自旋极化的节线

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摘要： 最近关于在β_{12}和χ_3硼烯中观测到狄拉克费米子的报道引起了人们极大的关注。基于第一性原理以及紧束缚模型，我们发现在β 硼烯中存在开放以及闭合两种类型的节线。这两种节线是由三条线性色散的能带交叉形成，同时受到时间反演对称性以及镜面对称保护。如果我们通过磁近邻效应破坏掉时间反演对称性，我们可以观测到原先的自旋简并的节线（节环）退化成完全自旋极化的节线（节环）。另外，垂直电场导致的Rashba 自旋轨道耦合效应使得自旋相反的电子态往相反的动量方向移动，从而在Γ 点附近形成了两个新的节环。

关键词：节线半金属 磁近邻效应 紧束缚模型

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S-P025

专题代号：S

Surface superconductivity in the type II Weyl semimetal $TaIrTe_4$

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abstract：The search for unconventional superconductivity in Weyl semimetal materials is currently an exciting pursuit, since such superconducting phases could potentially be topologically nontrivial and host exotic Majorana modes. The layered material $TaIrTe_4$ is a newly predicted time-reversal invariant type II Weyl semimetal with minimum number of Weyl points. Here, we report the discovery of surface superconductivity in Weyl semimetal $TaIrTe_4$. Our scanning tunneling microscopy/spectroscopy (STM/S) visualizes Fermi arc surface states of $TaIrTe_4$ that are consistent with the previous angle-resolved photoemission spectroscopy (ARPES) results. By a systematic study based on STS at ultralow temperature, we observe uniform superconducting gaps on the sample surface. The superconductivity is further confirmed by electrical transport measurements at ultralow temperature, with an onset transition temperature (T_c) up to 1.54 K being observed. The normalized upper critical field $h^*(T/T_c)$ behavior and the stability of the superconductivity against the ferromagnet indicate that the discovered superconductivity is unconventional with the *p*-wave pairing. The systematic STS, thickness and angular dependent transport measurements reveal that the detected superconductivity is quasi-one-dimensional (quasi-1D) and occurs in the surface states. The discovery of the surface superconductivity in $TaIrTe_4$ provides a new novel platform to explore topological superconductivity and Majorana modes.

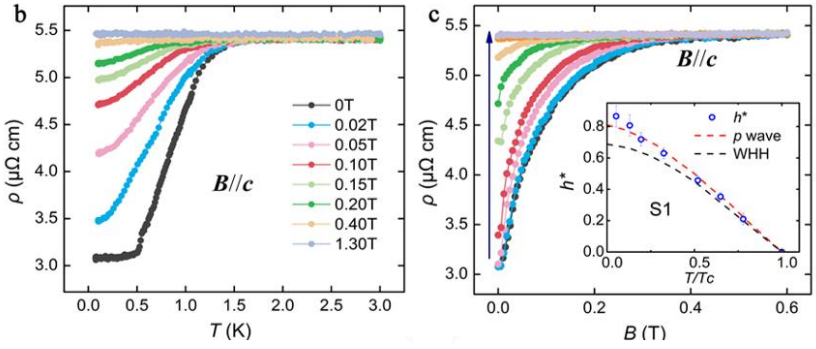

Figure1 Electric transport properties of $TaIrTe_4$ single crystal

Keywords：Surface superconductivity, type II Weyl semimetal

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【1】 Ying Xing et al, Surface superconductivity in the type II Weyl semimetal $TaIrTe_4$, *arXiv:1805.10883* (2018).
基金项目：This work was supported by the National Basic Research Program of China (Grant No. 2018YFA0305604, No. 2017YFA0303302, and 2016YFA0301604), the National Natural Science Foundation of China (Grant No. 11888101, 11774008, 11574095, 11704414, No. 11574008, and No. 11761161003), Beijing Natural Science Foundation(Grant No. Z180010), the Science Foundation of China University of Petroleum, Beijing (Grant No. 2462017YJRC012, 2462018BJC005) et al.

S-P026

专题代号：S

Prediction of nodal-line semimetals in two-dimensional black phosphorene

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摘要：Topological semimetals, with conduction bands and valence bands crossing each other near the Fermi level, are a new kind of topological electronic states, different from topological insulators. The degenerate energy points with zero-, one-, or two-dimensional manifolds can form topologically nontrivial Dirac/Weyl, nodal line, and nodal-surface semimetals, respectively. For the topological nodal-line semimetals, they can be divided into three categories according to the crystal symmetries owned: (1) the nodal-line protected by mirror reflection; (2) the nodal-line protected by inversion, time-reversal, and spin rotation symmetries; (3) the double-nodal line protected by twofold screw rotation, inversion, and time-reversal symmetries. Topology of the nodal-line semimetals can be identified by topological invariants, including Z_2 and Z etc.

In the present work, based on density function theory (DFT), we propose a two-dimensional topological nodal-line semimetals in layered black phosphorene (BP), which has attracted considerable interest recently. BP has potential applications in nanoelectronics owe to its high carrier mobility, high anisotropy, and negative poisson ratio etc exotic behaviors. We find that in the AA' bilayer BP with a certain biaxial compression strain, a closed nodal-line degenerate bands appears at the Fermi level and are protected by mirror reflection. The degenerate bands have opposite mirror eigenvalues ± 1 when spin-orbit coupling (SOC) is ignored. Drumhead-like edge states have been obtained along the Γ-X direction. Due to the weak intrinsic SOC of a phosphorus atom, a band gap less than 10 meV is opened along the node line in the presence of SOC, and the edge states are almost unaffected by SOC. Multilayers AA' stack BP，such as BP with four and six layers, are also found to be nodal-line semimetals, under even smaller biaxial compression strain, which are more accessible in experiments.

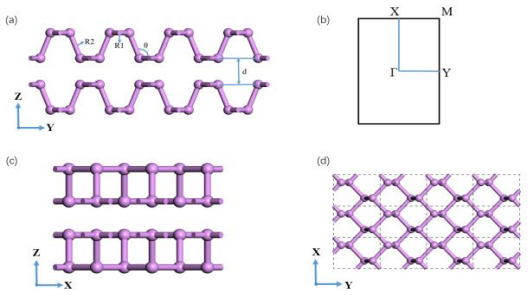

FIG. 1. Geometry structures of AA' bilayer BP.

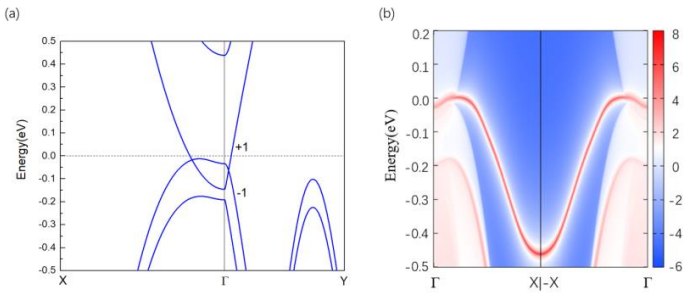

FIG. 2. Band structure and edge states for AA' bilayer BP.

Keywords: Crystal symmetry, Z topological invariant

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S-P027

专题代号：S

Twist投影的二维声拓扑绝缘体

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Abstract: Acoustic analogs of electronic or photonic topological insulators provide unique approaches to manipulate sound wave propagation. Inspired by twist-induced topological photonic insulators, here we propose a type of two-dimensional acoustic topological insulator (TI) via projecting a section of a three-dimensional twisting structure to a plane, assembling the projected meta-atoms into metamolecules, and arranging the metamolecules into unit cells to form a honeycomb lattice. It follows that in this acoustic TI, topological phases mimic pseudospin-up and pseudospin-down states, and the pseudospin-orbital couplings are tuned via changing the rotation angles of the meta-atoms, which eventually leads to band inversion. By calculating acoustic band structures, pressure field distributions, and spin Chern numbers of bands, we verify that the topological phase transition occurs around the double Dirac cone and present the topological phase diagram as a function of the rotation angle of the meta-atoms. Once the coupling between adjacent metamolecules is sufficiently strong, mode inversion of topological states emerges. Furthermore, we numerically demonstrate the existence of topologically protected edge states. It is shown that robust pseudospin-dependent one-way transmission is immune to defects at the edge of topological distinct regions, which can be applied to acoustic wave transmissions and communications. Our approach in acoustic systems provides a strategy to explore abundant topological states in two-dimensional systems.

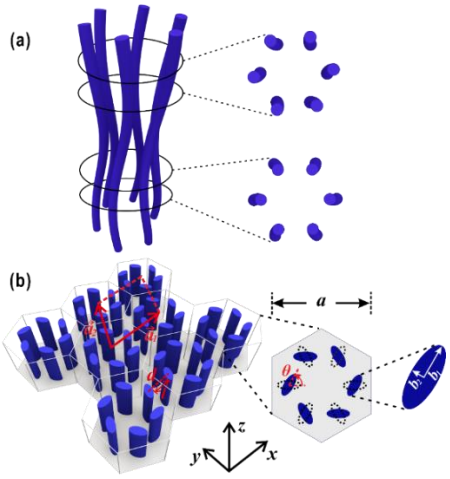

Fig.1. Schematic of the twisted wire bundle and their projections to xy plane.

Keywords：Acoustic topological insulator Topologically protected edge states
Unidirectional transport

Reference

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S-P028

专题代号：S

Searching the $Mn(Sb,Bi)_2Te_4$ family of materials for the ideal intrinsic magnetic topological insulator

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摘要：Quantum magnetic topological states combining the topological anomaly and magnetic order, such as quantum anomalous Hall (QAH) states, topological axion insulating states, and magnetic Weyl states, emerge rich exotic quasiparticles with or without counterparts to mimic real particles in universe, of which further in-deep studies and potential applications, such as the prestigious quantum device, are extremely limited by the lack of suitable intrinsic magnetic topological insulators (MTIs). Here, we grow single crystals of the $Mn(Sb,Bi)_2Te_4$ family as part of a search for intrinsic MTIs, and by combining the angle-resolved photoemission spectroscopy, low-temperature transport, and first-principles calculations, we investigate the band structure, transport properties, and magnetism, as well as the evolution of topological anomaly in this family of materials. All the materials could be exfoliated to produce two-dimensional flakes. Taking careful consideration of the multiple transition processes of charge carriers, magnetization, and topology, we conclude that there exists an ideal MTI zone in the $Mn(Sb,Bi)_2Te_4$ phase diagram, hosting a potential high-temperature QAH effect, as well as possible for device applications.

关键词： Magnetic topological, Topological insulator

参考文献：

【1】 Bo Chen *et al.*, Searching the $Mn(Sb,Bi)_2Te_4$ family of materials for the ideal intrinsic magnetic topological insulator, arXiv 1903.09934.

基金项目：National Key R&D Program of China (2017YFA0303203 and 2018YFA0306800), the National Natural Science Foundation of China (91622115, 11522432, 11574217, 11674165, 11227902, 11774154, 61822403, 11874203, U1732273 and U1732159), the Natural Science Foundation of Jiangsu Province (BK20160659), the Fundamental Research Funds for the Central Universities, Users with Excellence Program of Hefei Science Center CAS (2019HSC-UE007) and the opening Project of the Wuhan National High Magnetic Field Center.

S-P029

专题代号：S

Proximity-induced surface superconductivity in Dirac semimetal Cd_3As_2

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摘要：Cd_3As_2 is a three-dimensional Dirac semimetal with separated Dirac points in momentum space. In spite of extensive transport and spectroscopic studies on its exotic properties, the evidence of superconductivity in its surface states remains elusive. Here, we report the observation of proximity-induced surface superconductivity in Nb/Cd_3As_2 hybrid structures. Our four-terminal transport measurement identifies a pronounced proximity-induced pairing gap (gap size comparable to Nb) on the surfaces, which exhibits a flat conductance plateau in differential conductance spectra, consistent with our theoretical simulations. The surface supercurrent from Nb/Cd_3As_2/Nb junctions is also achieved with a Fraunhofer/SQUID-like pattern under out-of-plane/in-plane magnetic fields, respectively. The resultant mapping shows a predominant distribution on the top and bottom surfaces as the bulk carriers are depleted, which can be regarded as a higher dimensional analog of edge supercurrent in two-dimensional quantum spin Hall insulators. Our study provides the evidence of surface superconductivity in Dirac semimetals[1].

关键词：Surface superconductivity, Topological Dirac semimetal

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【1】 Ce Huang *et al*., Proximity induced surface superconductivity in Dirac semimetal Cd3As2, Nat. Comm.2019, 10. 2217

S-P030

专题代号：S

Topological Nonlinear Anomalous Nernst Effect in Strained Transition Metal Dichalcogenides

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摘要： Modern condensed matter physics is looks for new phenomena that arise from the properties of wave functions beyond the band structure of materials. A remarkable example of such phenomena is provided by local properties of wave functions, defined as the Berry curvature. The importance of Berry curvature is increasingly recognized in a wide range of areas in condensed matter physics, including anomalous Hall conductivities of ferromagnets, nonlocal transport and chiral optical responses in non-centrosymmetric metal and semiconductors. It is well known that the conventional Nernst effect requires broken time-reversal symmetry, namely there is no transverse charge current generated by a longitudinal temperature gradient in time-reversal symmetry materials as least in linear response regime. However, here we propose an emergence of nonlinear anomalous Nernst effect (NANE) as a second response to a temperature gradient in time-reversal symmetry but inversion broken materials. This non-linear thermoelectric effect origins from the Berry curvature of states near the Fermi surface and becomes a promising tool for understanding novel materials. Analogous to the nonlinear Hall effect, the largest symmetry of two-dimensional crystal that allows for nonvanishing NANE is a single mirror symmetry.

The C_{3v} symmetry of Nernst effect in transition metal dichalcogenides (TMDCs) with 1H structure would force the nonlinear current disappear. However, application of uniaxial strain can reduce this symmetry and leave only a single mirror operation. We investigate the non-linear Nernst effect in transition metal dichalcogenides (TMDCs) under the application of uniaxial strain. In particular, we predict that under fixed chemical potential in TMDCs, the non-linear Nernst current exhibits a transition from T^{-2} temperature dependence in low temperature regime to a linear T-dependence in high temperature.

Key word: Topological effect, TMDCs, Berry curvature, 2D materials, Anomalous Nernst effect

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S-P031

专题代号：S

Spin-orbit coupling induced robust spin-Seebeck effect and pure thermal spin currents in achiral molecule systems

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Abstract：Spin-Seebeck effect (SSE) is an effective route to realize pure spin current by using spin-polarized electrons or spin-wave transport in magnetic systems. Here we propose a route, i.e., by using spin-orbit coupling (SOC), to achieve robust SSE characterized by pure thermal spin current. The material examples are constructed on achiral nanotubes, and the theoretical results reveal that (i) as temperature gradient is applied along the nanotubes, thermal spin-up and spin-down currents with opposite flow directions are produced without any accompanying charge current, (ii) the SSE is robust against decoherence and nonuniform interchain SOC, (iii) the thermal spin currents display a multioscillation feature with increasing device temperatures, supporting their potential device applications in thermal spin-current multiswitcher, and (vi) strain engineering in the radical direction of nanotubes is an effective way to improve SSE and to control pure thermal spin current. These inspiring spin transport behaviors in achiral molecular systems put forward a mechanism to realize the robust SSE characterized by pure spin current and develop the research field of spin-orbito-caloritronics, which focuses on the interplay of electrons' spin and orbital degrees of freedom in the presence of temperature gradient.

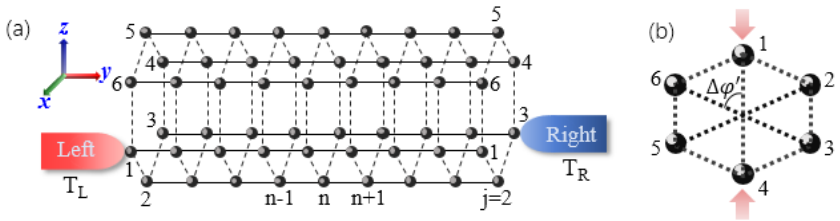

Fig.1.Schematic view of an achiral nanotube (no helical symmetry)

Key words：Spin-orbito-caloritronics, spin-orbit coupling (SOC), Spin-Seebeck effect

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基金项目：国家自然科学基金项目 No. 11774104 , No.11274128.

S-P032

专题代号：S

Categories of Phononic Topological Weyl Open Nodal Lines and a Potential Material Candidate: $Rb_2Sn_2O_3$

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摘要：The phononic topological Weyl closed nodal lines, including Weyl nodal rings, nodal chains, nodal nets, nodal links, and nodal knots, have been widely studied. The phononic topological Weyl open nodal lines (PTWONLs), however, have not been well investigated so far. By analyzing the coexistence of parity inversion and time-reversal symmetries, we found that the PTWONLs can be divided into three categories, with surface states hosting different shapes and positions in the Brillouin zone (BZ). Specifically, semiconducting $Rb_2Sn_2O_3$ was found to exhibit perfect PTWONLs in its phonon spectrum, which fills up one of the categories. Numerical calculations showed that the drumhead-like surface states exist on the (010) surface and six PTWONLs appear in the first BZ due to the C_3 rotation symmetry in the crystal structure. Their topological nontrivial nature was confirmed by calculating the Berry phase and by the linear phononic bands around the Weyl points. These theoretical findings provide a deep understanding into the phononic Weyl-open-nodal-line physics, and a promising candidate for experimental verification.

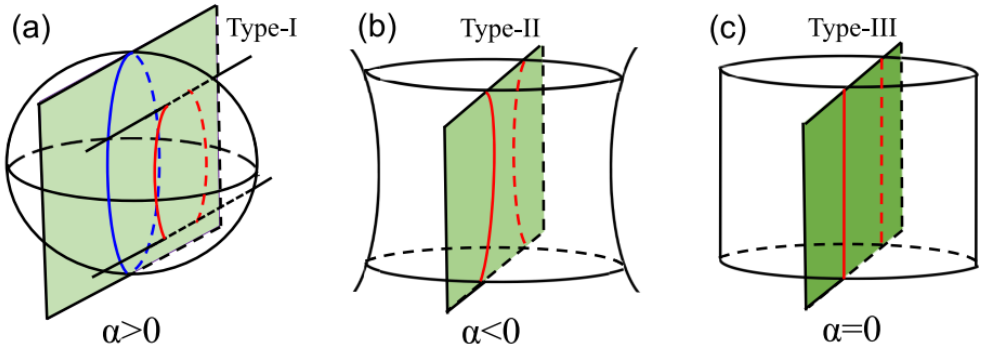

Figure 1. Definition of different topological Weyl open nodal lines with different parameters α, where the red dashed lines stand for the nodal lines. (a) Nodal rings or lines for α > 0. (b), (c) Nodal lines for α< 0 and α= 0, respectively.

Key Words: Phononic Topological Weyl Open Nodal Lines, Phonon Berry Phase, Drumhead-like Surface States, Fermi Arc, First-principle Calculations

【1】Qing-Bo Liu, Hua-Hua Fu*, Gang Xu, Rui Yu, and Ru-Qian Wu. Categories of Phononic Topological Weyl Open Nodal Lines and a Potential Material Candidate: Rb2Sn2O3. J. Phys. Chem. Lett. 2019, 10, 4045-4050.

基金项目：国家自然科学基金项目(No.11774104,11274128) DOE-BES (Grant No. DEFG02-05ER46237)

S-P033

专题代号：S

Interlayer quantum transport in Dirac semimetal $BaGa_2$

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Abstract: Quantum limit is quite easy to achieve once the band crossing exists exactly at the Fermi level (E_F) in topological semimetals. In multilayered Dirac fermion system, the density of Dirac fermions on the zeroth Landau levels (LLs) increases in proportion to the magnetic field, resulting in intriguing angle- and field-dependent interlayer tunneling conductivity near the quantum limit. $BaGa_2$ is an example of multilayered Dirac semimetal with anisotropic Dirac cone close to E_F, providing a good platform to study its interlayer transport properties. In this paper, we report the negative interlayer magnetoresistance (NIMR, I//c and B//c) induced by the tunneling of Dirac fermions on the zeroth LLs of neighbouring Ga layers in $BaGa_2$. When the field deviates from the c-axis, the interlayer resistivity $\rho_{zz}(\theta)$ increases and finally results in a peak with the field perpendicular to the c-axis. These unusual interlayer transport properties (NIMR and resistivity peak with B⊥c) are observed together for the first time in Dirac semimetal under ambient pressure and are well explained by the model of tunneling between Dirac fermions in the quantum limit.

Key words: quantum oscillations, electronic structure, the zeroth Landau level, first-principles calculation, angle-resolved photoemission spectroscopy

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国家重点研发计划 (批准号. 2017YFA0302903)
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