M 计算物理

分会召集人：赵纪军、刘正猷、龚新高、解士杰、林海青

M-001

专题代号：M

Computational design of functional nanostructures

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The discovery of graphene opened a door for manufacturing and investigating two-dimensional (2D) materials. After more than ten years of development, 2D materials have become one of the most important topics in materials research, with dozens of new materials having been synthesized experimentally and even more predicted theoretically. In this talk, I will talk about the design of 2D materials using density functional theory (DFT) based first principle calculations. Motivated by the experimental fabrication of a single atomic layer transition metal monochalcogenide (CuSe) with an intrinsic pattern of nanoscale triangular holes, the hole-free CuSe with honeycomb lattice is predicted to be endowed with the Dirac nodal line fermion (DNLF). This very rare DNLF state is evidenced by topologically nontrivial edge states situated inside the spin-orbit coupling gaps. Moreover, we found that the CuX (X=S, Se and Te) monolayers with honeycomb lattices are a group of highly p-doped semiconductor with a large bandgap above Fermi level. Remarkably, based on first-principles calculations, we successfully convert the semiconducting monolayer CuS and CuTe into topological insulators (TIs) by simply adsorbing Na and K respectively, and CuSe into a TI by adsorbing a mixture of Na and K. The transformation of a semiconductor to a TI is underlined by an orbital design principle that involves introducing an extrinsic s-orbital state into the intrinsic sp-bands of a 2D semiconductor, so as to induce s-p band inversion for a TI phase, as demonstrated by tight-binding model analyses. This approach can be applied to other 2D semiconductors. Our findings open a new door to the discovery of TIs by a predictive materials design, beyond finding a preexisting 2D TI.

I’d like to thank the Lei Gao, Jiatao Sun, H.-J. Gao in IoP, Yuyang Zhang at UCAS, Feng Liu at U of Utah.

关键词：CuSe, Topological insulator, 2D semiconductor, DFT, Computational design

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M-002

专题代号：M

基于对称性指标预测拓扑材料

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摘要：Although the richness of spatial symmetries has led to a rapidly expanding inventory of possible topological crystalline (TC) phases of electrons, physical realizations have been slow to materialize due to the practical difficulty to ascertaining band topology in realistic calculations. Here, we integrate the recently established theory of symmetry indicators of band topology into first-principle band-structure calculations and apply it to all non-magnetic compounds in the 230 space groups. An exhaustive database search reveals thousands of TM candidates. Of these, we highlight the excellent TMs, the 258 topological insulators and 165 topological crystalline insulators which have either noticeable full band gap or a considerable direct gap together with small trivial Fermi pockets. We also give a list of 489 topological semimetals with the band crossing points located near the Fermi level. All predictions obtained through standard generalized gradient approximation (GGA) calculations were cross-checked with the modified Becke-Johnson (MBJ) potential calculations, appropriate for narrow gap materials. With the electronic and optical behavior around the Fermi level dominated by the topologically non-trivial bands, these newly found TMs candidates open wide possibilities for realizing the promise of TMs in next-generation electronic devices.

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M-003

专题代号：M

New materials and new states under extreme conditions

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ABSTRACT

High pressure is an important method to modify the free energy surface of materials and overcome the barriers for synthesizing new functional materials. On the other hand, crystal structure search based on ab initio calculations has been successfully used to prediction new materials. In this talk, I will introduce some of our recent work on theoretical prediction on high pressure phase transitions, functional materials with interesting properties, and new states of matter under extreme conditions, such as superionic states.

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M-004

专题代号：M

Computational design of near room-temperature superconducting materials under pressure via CALYPSO code

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There is growing experimental evidence for novel electronic properties of dense hydrogen-rich materials under pressure. However, it is still highly required to search for superconducting materials with near or even above room temperature. We here explored several candidate structures for hydrides [1-3] under pressure using CALYPSO code [4, 5]. Electron-phonon coupling calculations predict the existence of new superconducting phases, some exhibiting superconductivity in the range of room temperature. Further analysis shows that the hydrogen-hydrogen bonding in superhydrides played a critical role in determining electron-phonon coupling parameters. Moreover, the calculated stabilities indicate the materials could be synthesized at pressures that are currently accessible in the laboratory. The results open the prospect for the design, synthesis, and recovery of new high temperature superconductors with potential practical applications.

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M-005

专题代号：M

Thermoelectric Transports in the Materials with Chemical Bond Hierarchy

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Searching for high-performance thermoelectric (TE) materials, after a very long-time struggle with the traditional crystalline semiconductors of narrow gap, seems to be halted in recent years. Even thermodynamics says no up limit on the TE figure of merit zT, reliable performance of practical materials always show limited zTs, still far away from the requirements of mess industrial applications. We recently proposed that complex materials with chemical bond hierarchy could be candidates of good thermoelectric materials. Our work showed that this types of materials exhibit specific part-crystalline part-liquid (PCPL) or part-crystalline part-amorphous (PCPA) structure, containing at least two different types of sublattices, one relatively rigid crystalline and another one strongly disordered. The former leads to interesting electrical transport, implying existence of an inherent electron conduction network, and the latter one results in extremely low lattice thermal conductivity, but different from the traditionally recognized minimum lattice thermal conductivity. This talk presents our work on surveying the general characteristics of transports in materials with chemical bond hierarchy.

M-006

专题代号：M

Half-Heusler 材料中的缺陷分布模拟及高通量筛选

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摘要：

立方结构的 half-Heusler (HH)材料因其优良的电子性质、热力学稳定性、价格低廉等特点在热电材料领域受到广泛关注，但是它的高热导率也限制了其热电性能的进一步提升。对于实验上发现的最好的 p 型 FeNbSb 材料，V 和 Ti 掺杂对于它的性能有着不同的影响。为了描述在实验条件下（温度和尺度）的缺陷分布情况，我们结合了团簇展开和蒙特卡洛方法。通过相图发现，在低温下 $FeNb_{1-x}V_xSb$ 倾向于相分离，但在 $FeNb_{1-x}Ti_xSb$ 中发现了稳定基态相；在高温下会形成固溶体。如果控制温度至相边界，会出现

固溶体和相分离的共存，可以同时有效的散射多种频率声子，进一步降低热导率和提高 FeNbSb 基材料的热电性能。另外，我们用 FeTiSb(17 电子体系)和 NiTiSb（19 电子体系）混合形成新的 18 电子体系，取代 18 电子的 CoTiSb，从而寻找具有本征低热导率的基态。低温下发现 $Fe_{1-x}Ni_xTiSb$ 倾向于形成稳定的基态相，在高温时形成固溶结构，其中 $Fe_2Ni_2Ti_4Sb_4$ 是具有 18 电子的半导体材料。进一步的理论计算发现理论预测的 $Fe_2Ni_2Ti_4Sb_4$ 体系是一种良好的热电材料（不但具有好的电学性能，而且本征热导率也较低）。我们进一步通过对 70 余种热力学稳定 HH 材料的电学和热学性能进行详细的计算，从中筛选出多种新型的 n-和 p-型的高效 HH 热电材料。

M-007

专题代号：M

Defect Control for Solar Cell Absorbers via First-Principles Calculations

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Defect properties are of crucial importance for solar energy materials. Shallow defects/impurities may act as carrier generators for n- or p-type semiconductors therefore facilitate carrier separation. However, deep ones may act as non-radiative recombination centers. In this talk, I will present our understandings on defects, including point defects and grain boundaries, in prevalent solar cell absorbers including GaAs[1], CdTe[2], CuInSe2[3,4], Cu2ZnSnSe4[5,6] and perovskite CH3NH3PbI3[7-9]. General trends have been observed through first-principles calculations: (i) the dominating defects in more covalent systems usually have higher formation energies but electronically deeper; (ii) antibonding coupling at valence band maximum i.e. pd coupling in CuInSe2 and sp coupling in CH3NH3PbI3, is able to result in defect tolerance. The trends explained diverse defect properties and defect engineering strategies among aforementioned solar cell absorbers and provided guidance for searching promising solar cell absorbers in future.

关键词：Defect; Semiconductor; First-Principles

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M-008

专题代号：M

Is Disordered Structure the Necessary and Sufficient Condition for Glass Transition

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For a long time, the intrinsic nature of glass states or glass transitions is a mystery. Recently, more and more studies tend to show that, a glass processes a relatively flat potential energy landscape. Undoubtedly, this conclusion is extremely important, however it only indicates that, the flat potential energy landscape is a necessary condition for forming glass states or occurring glass transitions. Is the flat potential energy landscape a sufficient condition for glass formation or glass transition? Here we prove for the first time that, a flat potential energy landscape is not only a necessary but also a sufficient condition for the formation of glasses. By adjusting the flatness of potential energy landscape, we have demonstrated that: (1) no matter how symmetrical the structure is, as long as the system is in a region of potential energy landscape deepen enough, it will undergo a first-order solid-liquid phase transition; and (2) as long as the system is in a region of potential energy surface flat enough, it will undergo glass transition, which is independent on its structural symmetry. For the first time, our molecular dynamics simulations uncover the direct transfer from one potential energy minimum to another below the glass transition temperature, which is the flat feature of potential energy landscapes. This kind of transfer is accomplished by a cooperative diffusion, which is a direct reflection of assumption for motions in metabasin and for chain-like motions of the Adam-Gibbs's entropy theory.

Key words: glass and glass transition, potential energy landscape, molecular dynamics simulation

M-009

专题代号：M

基于准二维材料的有效载流子掺杂调控和储能的物理机制

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以 MoS_2 为代表的准二维材料比表面积大、物理化学性质优异、力学稳定性高，同时具有良好的电学性能，因此在快速纳电子器件和储能领域的应用前景引人关注。针对单层半导体相的 $1H$-MoS_2，其本征的载流子浓度仅为~10^{10} cm^{-2}，为提高基于单层 $1H$-MoS_2 电子器件的驱动电流，如何在不引入带隙中缺陷能级的情况下，对其进行有效的载流子掺杂至关重要。在前期关于 MX_3 电子结构性质研究的基础上[1]，通过采用与 $1H$-MoS_2 晶格匹配良好、宽带隙、带边位置合适的单层 YBr_3 作为缓冲层，构建异质结，我们的理论研究结果发现，结合掺杂 Li、Na、K、Ca 或者 F 元素可以在 $1H$-MoS_2 中实现有效的 n 型或 p 型载流子掺杂，并且掺杂的稳定性得到提高[2]。针对可作为超级电容器的电极材料的金属相 $1T$-MoS_2，其赝电容和循环稳定性能良好。为了阐明其原子结构、电子结构和赝电容之间关系的物理机理，并有效调控其赝电容性能，我们的研究结果发现：在决定赝电容的两个因素中，电极材料与电解质中的 H^+ 之间的电荷转移量随着 H^+ 吸附浓度的增大线性增大；电极材料功函数的变化量也在逐渐增大，但是变化率却逐渐变缓，这与 $1T$-MoS_2 在吸附不同浓度的 H^+ 时呈现金属-半导体-金属转变的性质有关；同时通过引入本征缺陷硫空位，可以有效提高赝电容的性能[3]。上述研究结果，将为理解、设计和调控 $1H$-MoS_2 的载流子浓度和 $1T$-MoS_2 的赝电容性能提供重要的理论支撑。

本工作得到国家自然科学基金（11874223, 51871121）和国家重点研发计划（2016YFB0901600）的支持。

关键词：电子结构；载流子掺杂；储能机理；准二维材料；第一性原理计算

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M-010

专题代号：M

Stability of asymmetric polar or semipolar surfaces and edges

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Stability estimation of asymmetric polar or semipolar surfaces or edges is the most challenging problem in surface and low dimensional systems. With the recent development, we report highly accurate computational approaches that reduce the error from above 10 percent to less than one percent. Various systems such as III-V, II-VI, and two dimensional semiconductors are investigated. Combining with edge passivation and thermodynamic analysis, equilibrium shapes of BN are constructed and agree with experimental observation excellently.

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M-011

专题代号：M

多元低对称性半导体中点缺陷诱导的载流子非辐射复合

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The defect-induced non-radiative recombination is a serious limit to the minority carrier lifetime and the photovoltaic performance of the light-absorber semiconductors in solar cells. The accurate determination of the carrier-capture cross sections of defects and the corresponding carrier recombination rate is challenging for both the experimental measurement and theoretical calculation. Experimentally, there is no efficient and direct method for measuring the carrier-capture cross sections or non-radiative recombination rate induced by different point defects.

Usually the carrier lifetime was measured, but it is difficult to identify which defect dominates the non-radiative recombination process, especially for the multinary and low-symmetry which may have various point defects in the lattice. Through systematical defect search, we identified a series of possible recombination-center defects in three novel photovoltaic semiconductors, the quasi-one-dimensional Sb_2Se_3 and quaternary Cu_2ZnSnS_4. By combining the electron-phonon coupling effect and the static-coupling formalism, we calculated the carrier-capture cross sections of the possible non-radiative recombination-center defects in these semiconductors. These values are currently unavailable but critical for understanding the limiting factors of the minority carrier lifetime and simulating the photovoltaic devices. A simple empirical criterion was proposed for the quick identification of effective non-radiative recombination-center defects based on the calculated results, *i.e.*, the deep-level defects may have large carrier-capture cross sections if they are surrounded by strong bonds and undergo considerable structural relaxations after capturing a carrier.

*The work is finished in close collaboration with Menglin Huang, Jiqiang Li, Zhenkun Yuan, Prof. Xingao Gong and Prof. Su-Huai Wei.

M-012

专题代号：M

相变信息存储器的低功耗相变过程计算设计

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摘要：

相变信息存储技术因其速度快、数据非挥发已广泛应用于光盘储存，并是下一代应用涵盖从固态硬盘到内存最有竞争力的通用存储集成电路技术之一[1]。相变存储技术主要依赖于相变半导体的快速相变过程及新型存储材料的设计。然而，与其他主流存储技术相比，相变存储器的功耗几乎是最高的[1]，这限制了其在高密三维存储集成电路中的应用开发。功耗高一般认为是相变存储材料在数据存储时需要利用高能量电脉冲或者光脉冲实现高温熔化过程，从而实现电信号或光信号的显著转变。本报告介绍作者近年来基于原子尺度分析与设计思路在克服相变存储高功耗这一关键问题上的一些有益探索：1.理论提出过渡金属元素中心原子钉扎模型（如 Ti 掺杂 Sb_2Te_3 材料）来降低存储器功耗[2]；2.提出相变超晶格 GeSbTe 材料可通过位错运动触发电信号转变的低功耗存储过程[1,3]；3.探索发现相变存储半导体

GeTe 从菱方相到立方相的超快（非熔化）有序相变路径[4]。这些结果为低功耗相变信息存储器乃至高密度存储电路的工业开发提供有益参考建议。

关键词：相变存储技术 高密度三维存储集成电路 锗锑碲 超晶格 非熔化相变

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M-013

专题代号：M

光致相变材料的理论设计与计算研究

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关键字：密度泛函理论、光电场、马氏体相变

摘要：目前商用相变材料主要基于 Ge-Sb-Te 合金材料。这种材料具有两种局域稳定结构，即晶相和非晶相，它们的电阻值具有明显的差别。在光照加热下，晶相和非晶相之间可以相互转变，从而可以作为“0”和“1”两个态进行数据存储。然而，这样的相变属于重构型，其相变前后原子附近的拓扑结构没有明确关系，相变过程中原子的位移很大，需要打破很多化学键。因而相变所需能量较高。另一种相变，即位移型相变，是从有序相变为另一个有序相，需要较小的能量输入。为了设计新型微型结构相变材料，人们开始讨论二维材料的有序-有序相变。二维材料中的原子可以在 z 方向较自由地运动，从而相变过程中的应力集中问题可以被较好地解决。例如，过渡金属二硫化物（TMD，如 MoS_2）单层材料具有 2H 和 1T′ 两个相，理论和实验都证明了可以通过应变、锂化或者静电场的方式诱导 2H→1T′ 结构相变。然而，这些方案都需要和样品直接接触，这导致一个有趣的问题，能否用非接触式的光场来诱导二维材料的结构相变？我们将介绍一种新的相变方案，即通过讨论光电场对材料的影响，通过第一性原理计算线偏振光场下材料的自由能变化，预言光照下二维材料的快速结构相变。同时，我们还预言了一系列光诱导的拓扑相变。这一类相变属于马氏体相变，相变速度很快，能垒低，有利于作为新型的二维相变存储材料。

M-014

专题代号：M

Photoinduced Vacancy Ordering and Phase Transition in $MoTe_2$

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Abstract: We show that non-equilibrium dynamics plays a central role in the photoinduced 2H-to-1T' phase transition of $MoTe_2$. The phase transition is initiated by a local ordering of Te vacancies, followed by a 1T' structural change in the original 2H lattice. The local 1T' region serves as a seed to gather more vacancies into ordering and subsequently induces a further growth of the 1T' phase. Remarkably, this process is controlled by photogenerated excited carriers as they enhance vacancy diffusion, increase the speed of vacancy ordering, and are hence vital to the 1T' phase transition. This mechanism can be contrasted to the current model requiring a collective sliding of a whole Te atomic layer, which is thermodynamically highly unlikely. By uncovering the key roles of photoexcitations, our results may have important implications for finely controlling phase transitions in transition metal dichalcogenides.

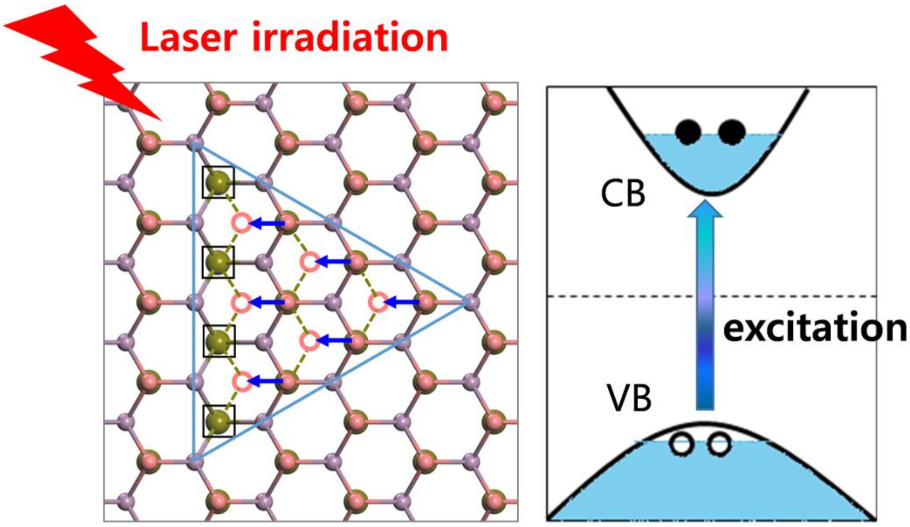

Figure1 Schematics for laser-induced phase transition in $MoTe_2$

Keywords：Non-equilibrium, excited state, vacancy ordering, phase transition, nucleation and growth

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M-015

专题代号：M

ABACUS 软件中高效杂化密度泛函计算的实现

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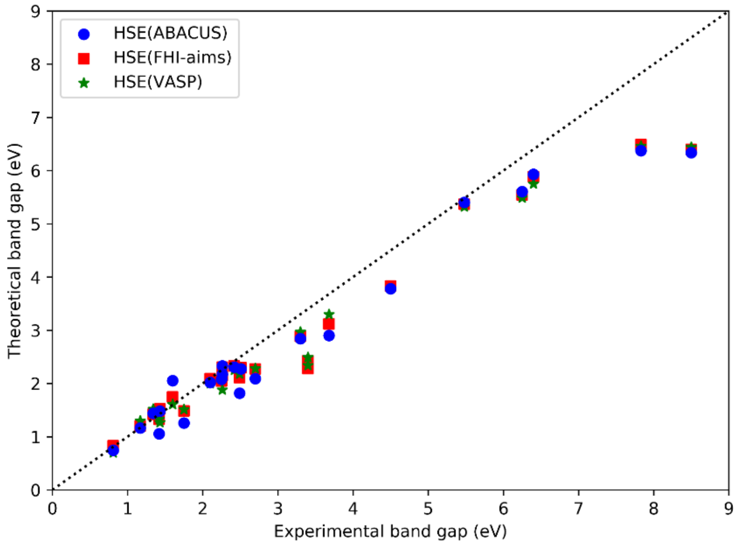
摘要： ABACUS (Atomic-orbtial Based Ab-initio Computation at UStc) 是中国科学技术大学量子信息重点实验室自主研发的基于原子轨道基组的第一性原理软件。在本报告中，我们介绍在 ABACUS 软件中高效的杂化密度泛函计算的实现。杂化密度泛函可以有效克服 LDA，GGA 等局域密度泛函近似带来的误差，提高计算精度，特别是改善能隙等物理量的计算准确性。但是杂化泛函需要计算严格的交换积分。该积分是一个四中心积分，直接积分计算复杂度高，是杂化泛函的计算瓶颈。我们采用 “resolution of identity” 方法，通过构建辅助基组，将四中心积分简化为双中心积分。利用原子轨道基组的局域性，我们可以实现四中心积分的计算复杂度随系统大小线性增长。我们在 ABACUS 中实现了这一算法。经过一系列算法（如对辅助基组的优化等）及程序实现的优化，我们很好的保证了程序的高效性，良好的可扩展性通过与 VASP 及 FHI-aims 等软件的对比测试表明计算结果准确可靠。目前， ABACUS 可以对千原子量级的物理系统进行高效、准确的杂化密度泛函计算。



图一 不同软件 HSE 计算常见半导体材料带隙与实验值的对比

关键词：ABACUS，杂化密度泛函，辅助基组

基金项目：科技部重点研发计划项目（NO. 2016YFB0201202）

M-016

专题代号：M

Manipulating quantum states by photoexcitation

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Photoexcitation is a powerful means in manipulating the states of matter, especially in complex quantum systems. As well-known charge density wave (CDW) materials, TaS_2 and $TiSe_2$ have been widely studied experimentally thanks to their intriguing photoexcited responses. However, the microscopic atomic dynamics and underlying mechanism are still under debate. Here we demonstrate photoexcitation induced ultrafast dynamics using time-dependent density functional theory molecular dynamics. We discover a novel collective mode induced by photodoping, which is significantly different from thermally-induced phonon mode. We also discuss photoinduced electronic phases in other two-dimensional materials such as phase inversion of CDW and Dirac state transition from type-I to type II. Our results provide a deep insight on coherent electron and lattice quantum dynamics during the formation and excitation of quantum electronic states.

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M-017

专题代号：M

基于群论图论的晶体结构预测新方法及其应用

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晶体结构是描述晶体材料的重要理论工具，在提升人类对材料的认知水平和应用水平方面发挥着极其重要的作用。计算机辅助的晶体结构预测和物性计算能够加速对新材料的研发和应用，在计算凝聚态物理和材料科学中都有着重要地位。近三十年来，随机策略、粒子群优化算法、遗传演化算法、模拟退火法、赝动力学模拟法、极小值跳坑法、基元拓扑法和周期性图论等晶体结构预测方法得到了很好的发展，并在晶体材料的预测方面取得了丰富的研究成果。标号商图作为另一种用于描述晶体材料的先进数学模型，能帮助我们记录晶体材料的拓扑特征和重现晶体结构，应该也能在对晶体材料进行研究的过程中发挥其重要作用。近年来，我们尝试结合标号商图和随机策略来进行晶体结构预测并开发了相应的晶体结构预测代码RG^2[**PRB, 97, 014104 (2018)**]。在本报告中，我们将介绍RG^2代码的产生背景、基本原理、工作流程和基本功能。另外，我们还将向大家展示RG^2在晶体结构预测中所取得的一些成功案例，包括最大带隙立方碳[**PRL, 121, 175701 (2018)**]，超级立方碳，具有幻数稳定性的二维石墨烯[**PRB, 99, 041405 (R), 2019**]，低能量的二维石墨相C_3N_4 **[Physica B, 562, 131 (2019)]**，新型低能量二维磷锗合金GeP，新化学计量比的二维磷锗合金Ge_3P_2，兼具高稳定性和Dirac节点线特征的二维硅薄膜，具有干净Dirac锥的新型二维$MoTe_2$等的发现。

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M-018

专题代号：M

无公度体系量子本征值问题的平面波方法

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摘要：无公度体系出现在许多前沿的领域中，例如二维电子材料、光子晶体、冷原子等，并带来了许多新颖的量子特性。但是周期性的缺失给理论计算和模拟带来了本质性的困难。在本报告中，我们对于无公度体系的电子结构相关本征值问题的计算提出了新型的数值算法：与传统的利用大的有公度超胞逼近无公度体系的方法不同，我们的算法在平面波的框架下直接离散本征值问题。随无公度特性出现的遍历性和从高维度的诠释带来了许多与周期性体系不同的性质。我们通过 1 维和 2 维的量子本征值问题的示例计算证明了我们方法的可靠性与高效性。此外我们还讨论了如何拓展我们的算法至更加实际的 Kohn-Sham 密度泛函计算。

关键词：无公度体系；量子本征值问题；平面波；密度泛函理论

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基金项目：国家自然科学基金 No. 91730302

M-019

专题代号：M

Quantum Monte Carlo Study of the Intermediate Phase in an Interacting Honeycomb Lattice with Staggered Potential

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By using the determinant quantum Monte Carlo method, we investigate the phase transitions in the ionic Hubbard model on the honeycomb lattice, varying the interaction strength and the difference in chemical potential on the two sublattices. Our exact numerical results reveal an interesting phase diagram where the electronic correlation may drive a band insulator metallic, and at a larger interaction, there is a second transition from metal to Mott insulator. It is also shown that the Mott insulating phase has antiferromagnetic long-range order at stronger interaction strength. A complete phase diagram is further achieved by studying the phase transition at large enough stagger potential and interaction strength, which shows that the intermediate state is more robust and occupies a large part of the phase diagram and that it should be more feasible to be detected experimentally.

M-020

专题代号：M

瓦尼尔函数在计算材料研究中的若干应用

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在对固体性质的理论研究中，人们习惯于在动量空间中理解固体的物理及化学特性。比如，动量空间下电子的色散关系，即能带结构，决定了电子输运，磁性等重要物理特性。动量空间下声子的色散关系，即声子谱，决定了晶格振动和热学的相关特性。动量空间下导体的费米面结构和拓扑对理解和研究强关联体系的新奇物性如超导，CDW，SDW 等有重要的作用。然而，在很多时候，固体的一些物理、化学特性与电子在实空间的局域性质有着密切关系。瓦尼尔函数为我们提供了一个在实空间研究电子局域性质的有力工具。我们最近基于最局域瓦尼尔函数方法在铁电，催化，以及重费米子领域展开了有关研究。这些研究展示瓦尼尔函数在计算材料研究中的重要价值，有望对其它方向的研究带来启发。

关键词：瓦尼尔函数；轨道物理；铁电性；重费米子；表面催化

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资助项目：国家自然科学基金河南省联合项目(No. U1804130)

M-021

专题代号：M

温稠密物质特性的第一性原理分子动力学研究

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摘要：温稠密物质介于凝聚态物质和等离子体之间，是武器物理、惯性约束核聚变（ICF)、天体物理等高能量密度科学与工程领域中物质存在和发展的重要阶段。其密度范围从通常固体密度到数十上百倍固体密度，温度从数千摄氏度到数十上百万摄氏度，其电子-电子、离子-离子及电子-离子之间的长程或短程相互作用产生的各种量子或经典意义上的竞争-协同效应极其多样，目前缺少有效的理论模型，实验数据也极端匮乏，研究具有挑战性。围绕温稠密物质的状态及诊断，报告人将系统介绍相关研究背景、研究现状及团队目前取得的理论进展。

M-022

专题代号：M

Design of functional semiconductors by knowledge-based materials screening

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摘要：Semiconductor materials are widely used in many optoelectronic applications such as solar cell, photo-detector, light-emitting diode, photocatalysis, etc. Discovery of new optoelectronic semiconductors via rational design is of crucial importance for making breakthrough enhancement of materials performance in applications. With dramatically increasing computing capability of supercomputers and continuously developed computational algorithms, people can resort to materials simulation to explore the properties of thousands of potentially useful materials in a fraction of time that the real experiments might take. This makes theoretical design of functional materials with desired properties in computers come true. In this talk depending on time I will present our development on open-source Python framework designed for large-scale high-throughput energetic and property calculations, the Jilin University Materials-design Python Package (Jump^2) and our recent work on design of functional semiconductors by knowledge-based materials screening.

关键词：新材料设计，高通量计算，机器学习

资助项目：中组部青年千人计划，科技部重点研发计划（2016YFB0201204），国家自然科学基金优秀青年基金（61722403）

M-023

专题代号：M

新型层状材料 PS_2 的理论和实验研究

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摘要：近年来，范德瓦尔斯层状材料引起凝聚态物理学等多学科领域的广泛关注[1]。最近，课题组团队采用晶体结构预测方法与高压实验合成相结合的方法以 P-S 系统为例证实 VA-VIA 族间可形成层状材

料，丰富了范德瓦尔斯层状材料数据库[2,3]。P-S 系统在环境条件下存在复杂的相图，热动力学稳定的化合物主要以分子晶体的形式存在。我们的理论计算表明在大约 8 GPa 的压力下，P 和 S 可以形成层状的范德瓦尔斯材料 PS_2。PS_2 具有 3R-MoS_2 结构（空间群，R-3m），实验合作者成功地在实验中观测到 PS_2 的存在。进一步的电子特性研究表明：PS_2 是金属并呈现出超导电性。在零压下，超导转变温度 T_c 为 11.3 K，随着压力增加 T_c 降低。不同于其它类 MoS_2 层状材料，单层 PS_2 具有比块体稍弱的电-声耦合强度，使得单层 PS_2 的 T_c 稍低于块体情况。这些研究结果为基于主族元素设计层状材料提供了参考，为新超导薄膜材料设计提供了研究平台。

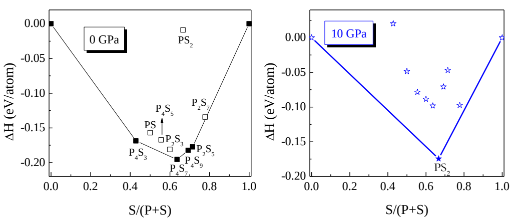

图 1 Convex hull of P-S system

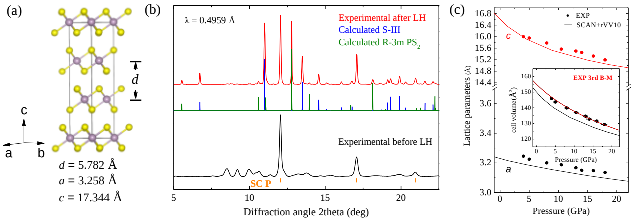

图 2 晶体结构，,XRD，晶格常数随压力变化和状态方程

关键词：结构预测 第一性原理 高压合成 超导

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M-024

专题代号：M

高压下的新型碳酸盐

董校

高压作为一个重要的极端条件，在物理、化学、材料等研究领域引发许多常压下难以观测到的新奇现象。碳循环是重要的研究内容。现在人们对地表的碳循环已经有了比较深入的研究，但是对地球深处的碳循环还知之甚少，甚至连高温高压下含碳化合物的存在形式都没有完全的了解。地表环境中，CaCO3 是岩石圈最主要碳源。我们通过结构预测的方

法来探索 Ca-C-O 三元体系在高压下出现的新的物质存在形式，发现两种新型的碳酸盐 Ca_3CO_5 和 CaC_2O_5，理论生成压力分别为 11 GPa 和 33 GPa。Ca_3CO_5 为 CaO 和新型原碳酸盐 Ca_2CO_4 的结合体，CaC_2O5 为碳酸根 CO_3^{2-}和 CO_2 分子的聚合产物。此类新型化合物证明高压下碳酸钙具有更强的储碳能力，同时在特定压力(33 GPa)下可以释放出 CO_2，促进人们对地球内部深碳循环的理解，发展和完善碳酸钙体系的相图和应用。

M-025

专题代号：M

Strain in van der Waals epitaxy and evidence of collective macroscopic effect of a negligibly small perturbation

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Recent studies of van der Waals heterostructures involving transition metal dichalcogenide (TMD) overlayers have revealed the formation of highly ordered mirror twin boundaries (MTBs) dividing domains in single 2H phase. Here, using a multi-scale modeling approach we identify that the MTB network formation results from a delicate interplay between strain accumulation in the heterostructure and single crystal preference of the growing overlayer. We determine the energy costs for the creation of the MTB by first-principles calculations, from which we show that even the presence of a perceived-to-be negligible strain is able to induce the formation of the MTB networks as an effective strain relief mechanism of the growing TMD monolayers, as observed experimentally. This counterintuitive finding demonstrates the importance of collective effects in weakly-interacting systems, i.e., in van der Waals epitaxy.

关键词： 2D 过渡金属硫化物；纳米有序网格；范德瓦尔斯外延；应力

M-026

专题代号：M

Emerging electronic states in van der Walls hetero-bilayers

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Bilayer heterostructures have received tremendous attentions in recent years. It is usually believed that electronic structures of stacked van der Waals (vdW) bilayers are simply superposition of their monolayer electronic structures. Here, we show that significant interlayer electronic hybridization occurs even for the most weak-interlayer coupled MoS$_2$/WSe$_2$ bilayer among MoS$_2$/WSe$_2$ [1], MoSe$_2$/PtSe$_2$ [2] and PtS$_2$/PtSe$_2$ [1] bilayers. Several interface states originating from the interlayer S-Se or Se-Se hybridization (illustrated in Fig. 1) are explicitly identified by our density functional theory calculations of up to 4000 atoms and confirmed by electrostatic force microscopy (EFM) imaging. In addition, our results also explained the found emerging states within the bandgap of the MoS$_2$/WSe$_2$ bilayer.

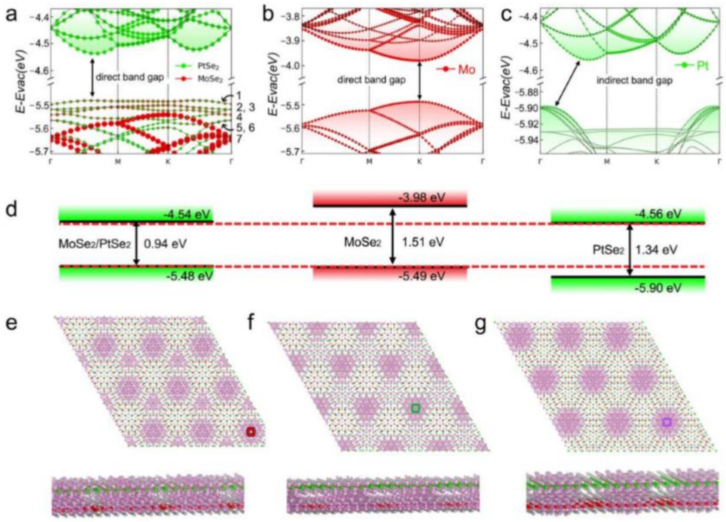

Fig. 1 Band alignment and Spatial structures of wavefunctions for PtSe$_2$ (1T)/MoSe$_2$ (1H) vertical heterostructures

Keywords：hetero-bilayer；interlayer coupling；gap state

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M-027

专题代号：M

Anomalous Dirac Plasmons in 1D Electrides

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Plasmon opens up the possibility to efficiently couple light and matter at sub-wavelength scales. In general, the plasmon frequency is dependent of carrier density. This dependency, however, renders fundamentally a weak plasmon intensity at low frequency, especially for Dirac plasmon (DP) widely studied in graphene. Here we demonstrate a new type of DP, excited by a Dirac nodal-surface state, which exhibits an anomalously density-independent frequency. Remarkably, we predict realization of anomalous DP (ADP) in 1D electrides, such as Ba3CrN3 and Sr3CrN3, by first-principles calculations. The ADPs in both systems have a density-independent frequency and high intensity, and their frequency can be tuned from terahertz to mid-infrared by changing the excitation direction. Furthermore, the intrinsic weak electron-phonon coupling of anionic electrons in electrides affords an added advantage of ultra-low phonon-assisted damping and hence a long lifetime of the ADPs.

M-028

专题代号：M

Innovations of 2D Multiferroics

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Multiferroic materials with coupled magnetism and ferroelectricity, even though scarcely exist in nature, are highly desirable for efficient “electric writing + magnetic reading”. For most current traditional multiferroics with strong magnetoelectric coupling, their practical applications are hindered by their weak polarizations and magnetizations. Here we show first-principles evidences that strong magnetoelectrics can be realized in a series of 2D multiferroics: in some bilayer systems, their “mobile” magnetism can be controlled by ferroelectric switching upon external electric field, exhibiting either “on” state with spin-selective and highly p-doped channels, or “off” state insulating for both spin and electron transport, which renders efficient electrical writing

and magnetic reading; vertical polarization can be maintained against depolarizing field, rendering high-density data storage possible; moreover, all those functions can be directly integrated into a 2D wafer, like n/p channels by doping in a silicon wafer. In some 2D systems, the magnetization can be switched by 90 or even 180 degree upon ferroelectric switching.

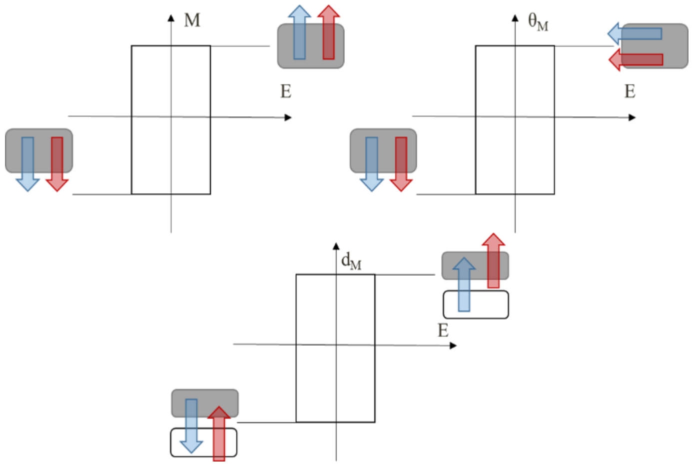

Fig.1 Several types of multiferroic coupling in 2D

Keywords：2D multiferroics；magnetoelectric coupling; first-principles calculations

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M-029

专题代号：M

具有优异的抗氧化性和高载流子迁移率的二维半导体

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具有合适大小的直接带隙、高载流子迁移率和良好的空气稳定性的二维半导体特别适合于材料的应用。层状金属氧化物由于其天然丰度、本征带隙和化学惰性，在二维材料中已成为一种新兴的材料。在第一性原理计算的基础上，我们系统地研究了 18 种单层金属氧化物的原子结构、能量稳定性和电子性能。所有这些单层金属氧化物都表现出优异的化学惰性，具有适度到宽的带隙（1.22～6.48 eV）和高的载流子迁移率（尤其是高达 8540 cm^{2}V$^-$

$^{1}s^{-1}$ 的 InO 单层），从而使这些低维材料有希望成为载流子运输的候选材料。这些二维金属氧化物在紫外波段表现出明显的吸收，吸收系数为$> 10^5\ cm^{-1}$。

通过第一性原理计算系统研究了完美的和带缺陷的单层三族硫属化物的氧化行为，发现完美的三族硫属化物单层表现出优异的抗氧化性，对氧气分子的解离和化学吸附具有较大的活化势垒，其值为 3.02~3.20 eV；相比之下，存在 S 或 Se 缺陷的三族硫属化物单层易受氧气的影响，对氧气分子的化学吸附仅有 0.26~0.36 eV 的活化势垒。有趣的是，将一个氧气分子填充到单层三族硫属化物的硫族空位中，可以保持完美体系的电子能带结构—带隙几乎完好无损，载流子有效质量只受到中等程度的干扰。

从理论上预测了硫化亚铜的一个层状新相 Cu_2S，称为 δ-Cu_2S，它具有新颖的电子特性和优异的抗氧化性。与已知的 β-Cu_2S 相相比，单层和双层 δ-Cu_2S 具有更低的形成能，δ-Cu_2S 相对于 β-Cu_2S 的较高稳定性表明 δ-Cu_2S 的实验合成具有很高的可能性。值得注意的是，δ-Cu_2S 表现出优异的抗氧化性，因为 δ-Cu_2S 上 O_2 的化学吸附具有 1.98 eV 的高活化势垒。在电子性质方面，δ-Cu_2S 是一种具有适中直接带隙（1.26 eV）和超高的电子迁移率（6880 $cm^2V^{-1}s^{-1}$）的半导体，约为 β-Cu_2S 双层的迁移率（246 $cm^2V^{-1}s^{-1}$）的 27 倍。

M-030

专题代号：M

二维过渡金属硫族半导体的缺陷控制与光电特性研究

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二维过渡金属硫属化合物因为其独特的原子结构和优异的光电性质在纳米电子和光电子器件领域展现出巨大的应用潜力。然而,二维过渡金属硫族化合物材料的光电性质强烈受其缺陷浓度和类型的影响。发展有效的方法去控制这些材料的缺陷是实现其在光电器件上应用的关键问题之一。本文结合第一性原理计算和实验表征技术系统研究了二硫化钼(MoS_2)、二硒化钼($MoSe_2$)和二硫化钨(WS_2)等二维过渡金属硫族半导体的可控制备、点缺陷的生长参数调控以及缺陷对光电性质的影响。研究结果显示：(1) 硫族空位的形成会引入较深的缺陷能级，极大地降低了它们载流子的输运和发光性能；为此，我们提出通过卤素钝化的方式去降低MoS_2和$MoSe_2$的空位缺陷浓度，可以达到提高电学输运和发光性能的目的；(2) 通过生长参数控制单层WS_2不同缺陷结构的形成，进而可以实现其发光特性的宽光谱调制；(3) 通过缺陷工程，在$MoSe_2$和VS_2中引入硫族空位和边缘缺陷去改变其局域的配位环境，可以实现对这些材料的费米能附近电子态的调控，从而在电催化制氢上表现出极佳的催化活性。

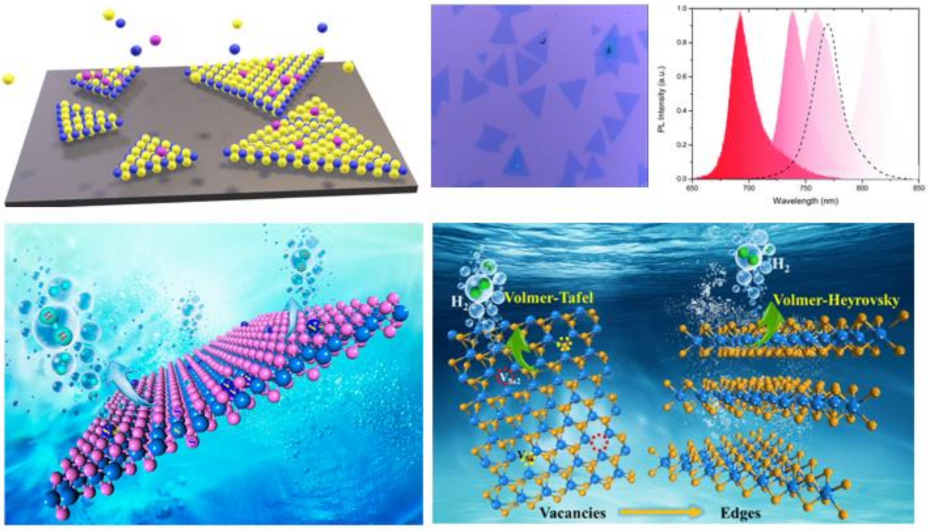

Fig. 1 二维过渡金属硫族化合物的缺陷形成、缺陷修复及其与发光和催化性质相互关系的研究成果示意图。

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M-031

专题代号：M

Theoretical studies on excitonic properties of 2D group-IV monochalcogenides

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Abstract: In this talk, I will present our theoretical investigation on excitonic properties of group-IV monochalcogenides (MX, M = Ge or Sn; X = S or Se). First, monolayer β-phase MX are shown to possess saddle-points in both the bottom conduction and top valence bands, and the positions of both saddle-points are close to their relative band edges. Due to the saddle-point exciton absorptions, a remarkable absorption peak within the fundamental gap is observed in these

materials. Importantly, the strong optical absorbance induced by saddle-point exciton absorptions and the appropriate band gap make monolayer β-GeSe and β-SnSe promising for solar cell applications with power conversion efficiencies as large as 1.11%.[1] Second, a new stable γ-phase MX is discovered and shown to have Camel's back band structure, and their influences on excitonic properties are discussed.[2]

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M-032

专题代号：M

Synergetic Role of Charge Transfer and Spin Selection in CO Oxidation on Two-Dimensional Half-Metallic Organic Frameworks

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ABSTRACT: Exploration of the interactions between the adsorbed species and reactive sites in heterogeneous catalysis is crucial in understanding the microscopic mechanism of the catalytic reactions. Here, using first-principles calculations within density functional theory, we predict that the two-dimensional ferromagnetic metal organic framework of $Mn_2C_{18}H_{12}$ can serve as a highly efficient catalytic platform for CO oxidation via a delicate synergetic effect of the charge transfer, provided by the hosting Mn atom, and spin selection preserved by its nearest neighboring Mn atoms. For the crucial step of the O_2 activation, the nearest neighboring Mn atoms are found to possess small charge transfer but significant magnetic moment changes, which ensures the spin-selection rule, thereby facilitating the adsorption of the spin-triplet O_2. For the reaction of CO with the activated O_2, we show that the reaction cycle can readily proceed via the L-H mechanism in the rate-limiting step with a relatively low reaction barrier, which can be further lowered by the adsorption of additional O_2 on the nearest neighboring Mn atoms. Furthermore, we examine the O_2 adsorption on $Mn_2C_{18}H_{12}$ (X represents 3*d* transition metal elements) derivative family, and identify that such an elegant synergetic phenomenon is also valid for the cases of X= Mn, Fe, Co, and Ni. Our findings may offer an avenue towards design of highly efficient magnetic catalysts for various important oxidation reactions wherein spin selection may be dominated.

Key words: Single atom catalyst; Charge transfer, Spin Selection, Synergetic Effect.

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M-033

专题代号：M

有机太阳能电池内非均匀场驱动的电荷分离机制

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摘要：Charge separation at donor/acceptor (D/A) interfaces plays a crucial role in the operation of photovoltaic polymer solar cells (PSCs), but the underlying mechanism still remains debated. Here, we present a model study to demonstrate how charge separation is achieved from a “cold” charge-transfer (CT) state in the presence of a nonuniform electric field or a nonuniform molecular-packing-configuration field. For the former case, we find that a “cold” CT state experiences two kinds of evolution paths, which are determined by the field strength of positions where the “cold” CT state is initially generated. In strong-field positions, the “cold” CT state is directly dissociated into free charges, while in weak-field positions, before the desired charge separation, the “cold” CT state experiences an ultrafast migration process along the D/A interface. As for the migration mechanism of the “cold” CT state, we attribute it to a driving force as a result of the different strength of electric fields felt by the negative charges and positive charges in the “cold” CT state. For the latter case, we find that the molecular-packing-configuration near the transition region from “D/A intermixed domain” to “D or A pure domain” can also provide a driving force to separate the “cold” CT state into free charges. In both cases, charge separation takes place in a timescale less than 300 fs, which might contribute to the ultrafast charge separation reported experimentally in high-performance PSCs. Our results also indicate that ultrafast and high-efficient charge separation in PSCs can be further promoted by optimizing the aggregation or crystallinity of acceptor molecules.

关键词：有机半导体 光伏过程 电荷转移态 非均匀场

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M-034

专题代号：M

催化性能提升与表界面结构调控

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摘要：

通过理解材料特性和形态之间的重要关系，纳米尺度模拟和表征为发现许多新颖的功能材料提供了可能。通过对电化学催化材料的催化机制的深入研究，开发新型高效率催化材料，优化催化剂组成和结构，降低过电位优化材料性能，是电解水催化材料研究的核心，是国际上制备高效经济制氢的研究工作重点之一。开发基于廉价原材料的具有高催化性能的氧析出反应（OER）催化剂成为氢能源应用里的关键一环。近来，实验中发现了过渡金属磷化物（$Ni_{12}P_5$）具有 OER 活性 $^{1-2}$。同时，贵金属的加入形成纳米核壳结构（$Au/Ni_{12}P_5$ 核壳结构）亦可以提升材料的催化能力。

利用从头计算方法，通过构造 $Ni_{12}P_5$ 不同表面结构，分析其稳定性，提出表面控制的方法；结合反应过渡态分析的方法，比较了不同表面该类化合物催化反应的过程，分析了 OER 反应中速率控制因素。同时也分析了贵金属元素通过界面对体系的原子结构和电子结构进行调节对催化性能的影响，为深入

认识过渡金属化合物结构和稳定性，如何通过表界面调控，提升特定反应的催化性能提供了参考。

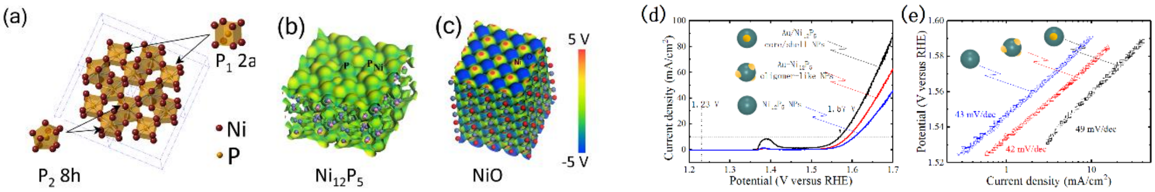

图 1 具有 OER 催化性能的 Au@Ni$_{12}$P$_5$ 核壳结构 [2]

关键词：第一性原理计算、氧析出反应（OER）、过渡金属化合物、表界面调控

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M-035

专题代号：M

具有超长载流子寿命的 MoSSe 纳米管用作光催化剂分解水

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摘要：半导体做光催化剂用于分解水产氢这一技术自 1972 年提出以来获得了极大得关注。然而，目前这一技术的效率很低，难以满足实际需求，限制了它的广泛应用。因此开发新型的高效光催化剂就显得非常重要。造成太阳光转化效率低的主要原因是是催化剂的光吸收效率以及载流子利用率极低。相比于传统的光催化剂，低维材料由于其比表面积大，表面态丰富和电子结构易调控等特性使得其有潜力解决上述问题并成为高效的光催化剂。最近，以二硫化钼为代表的过渡金属硫化物被实验证实是一种很有潜力的光催化剂。但是其光生载流子的复合几率很高，在一定程度上限制其使用，因此通过各种方法提高其光催化性能的研究具有重要的意义。

我们课题组基于含时密度泛函理论和非绝热分子动力学，预测了一维 MoSSe 纳米管是一种很有潜力的光催化材料。我们的计算结果表明，这种纳米管有合适的直接带隙，并且带边位置满足光催化分解水的要求。此外，在可见光波段内这种纳米管展现出优异的光吸收性能。最重要的是，本征的内建电场使得这一体系拥有

超长的载流子寿命（33 ns），这一数值是和最常见的光催化剂 TiO_2 相当的。超长的载流子寿命能够有效的降低电子空穴复合几率，从而提高光催化效率。因此，具有这些优异特性的 MoSSe 纳米管有巨大的潜力用作光催化剂分解水。

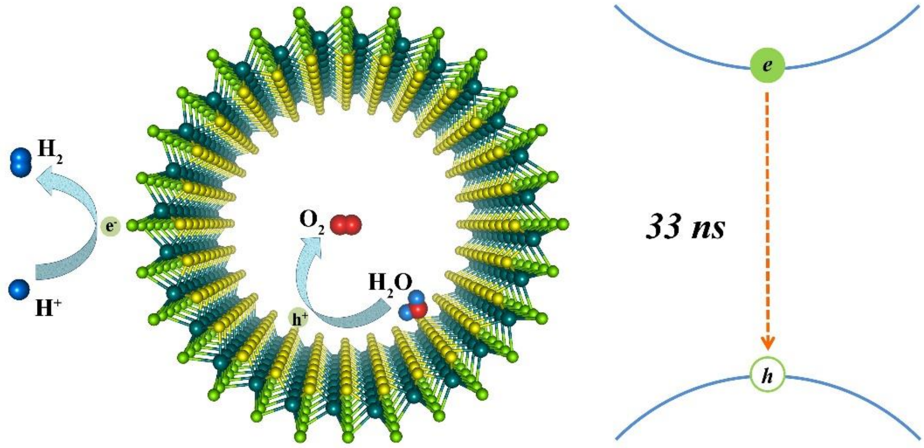

图 1 MoSSe 纳米管的光催化机制

关键词：第一性原理，光催化，载流子寿命

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M-036

专题代号：M

Metal Oxides Photocatalysis: From Single Molecular to 2D Amorphous Monolayers

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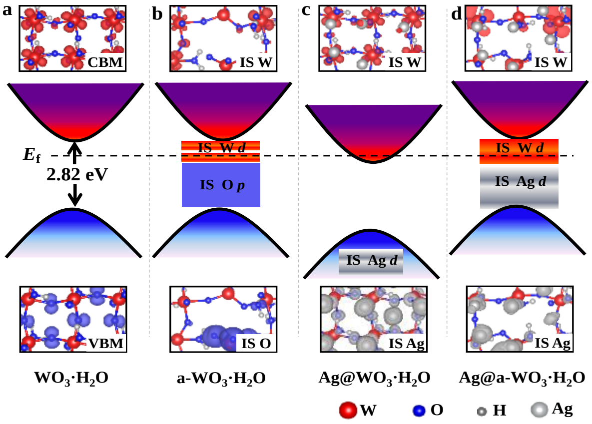
Abstract:
Designing of high efficient catalyst with non-noble metal is urgent and challenge. In this talk, I will discuss two types of designed catalysts that recently have realized in experiment. The first type of catalyst is single metal oxide WO_3, which is initially proposed in theory by filtering of hydrogen bond between crown molecule and WO_3, and then realized in experiment, showing high performance in degradation of organism. The second type of catalyst is Ag loaded WO_3 amorphous,

which shows excellent performance in oxygen reduced reaction (ORR). The underling mechanism could be attributed to the cooperative d-d coupling mechanism in amorphous effect. Specifically, the d state of Ag shift up ward, while the one of W state shift down ward, resulting to the oxygen reduced potential residing in the cooperative d states. The other case of amorphous catalyst is MO_3, where the second localized Anderson state of amorphous MO_3 resonates strongly with the N_2 molecule, giving rise to high performance of Nitrogen reduced reaction (NRR). Our proposed two types of non-noble metal oxides here might help to realize truly stable, high efficiency and economic catalyst.



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[3] Chong Li et al., Submitted

M-037

专题代号：M

杂发光系统中的暗激子态

李晓光

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等离激元光子学是围绕表面等离激元的原理和应用的学科，这一元激发可以与电磁场强烈耦合，使得我们可以通过纳米尺度结构接收，调控和辐射微米尺度光信息，并由此衍生出等离激元光子学的诸多应用。我们将回顾等离激元研究中的计算方法，同时介绍近年来，

我们在金属等离激元和分子/半导体激子的耦合体系中的一系列研究结果。此外，我们将介绍最近对暗激子态与等离激元相互作用体系的研究。

关键词：

等离激元，纳米光学，光与物质相互作用

M-038

专题代号：M

Excitonic Insulators in Direct-Gap Solids

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Direct-gap materials hold promises for excitonic insulators which possess a many-body ground state characterized by the spontaneously formed exciton condensate. In contrast to indirect-gap materials, here the difficulty to distinguish from a Peierls charge density wave is circumvented. However, direct-gap materials still suffer from a divergence of polarizability when the band gap approaches zero, leading to a diminishing exciton binding energy. We propose that one can decouple the exciton binding energy from the bandgap in materials where band-edge states have the same parity. First-principles calculations of two-dimensional GaAs and experimentally mechanically exfoliated single-layer TiS_3 and $1T$-MX_2 (M = Co, Ni and X = Cl, Br) lend solid support to this principle. Our study also provides new physical insights exploiting the multifaceted nature of charge gap, magnetism, and spontaneously-formed exciton condensate.

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M-039

专题代号：M

反铁磁薄膜中的千兆赫兹自旋波传输

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反铁磁自旋波的频率通常在太赫兹范围内，远高于铁磁体中的千兆赫兹自旋波。令人惊讶的是，最近的研究发现，夹在铁磁体（FM）与非磁金属 (Pt)间的反铁磁（AFM）薄膜，可有效传输千兆赫兹微波共振场驱动的自旋波。通过对铁磁体钇铁石榴石（YIG）和 AFM NiO 构成的异质结的第一原理计算及微观磁动力学模拟，我们发现千兆赫兹自旋角动量能够在 AFM 膜中有效传输。其原因是，YIG/NiO 界面存在较强的自旋交换作用，异质结在微波场中以驻波形式激发的自旋角动量能够以相干输运的方式有效在 NiO 中传输。我们还发现 NiO 中自旋角动量的传输特性及自旋流的大小，与 NiO 的磁各向异性、NiO/Pt 界面的阻尼密切相关。我们的研究结果为增强自旋电子器件中的自旋扭矩/电流产生提供了新的途径。

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M-040

专题代号：M

Computational Crystal Growth of Borophene

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Abstract:

Two-dimensional materials have attracted many attentions due to their unique physical and chemical properties since the discovery of graphene in 2004. Both experimental and theoretical studies suggest these 2D nanosheets are promising candidates for various applications, such as energy storage, catalysis, and medicine. To fully realize their potential in practical applications, high-quality large-area samples are required in a simple and low-cost way. As an atomically thin two-dimensional (2D) boron layer, borophene was recently synthesized on metal substrates and attracted a lot of attention due to its great potential for future applications. In this talk, we will report our recent findings on the structure, stability, and nucleation mechanism of boron clusters B_N ($N \leqslant 98$) and sheets on weakly interacting substrates using first-principles calculations and *ab initio* molecular dynamics simulations. We identified that by using a simple effective potential well, borophene can be grown on various weakly interacting substrates, including graphene, BN, BCN, and Bi_2Te_3. Our findings not only pave the way for the experimental growth of borophene but also provide a general methodology of investigation of the structure and stability of 2D elemental monolayers on chemically inert substrates.

M-041

专题代号：M

有机发光二极管热活化延迟荧光机制中的激子单三态演化研究

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有机发光二极管的一个重要发光机制是热活化延迟荧光。在这个机制中的关键过程是激子或者电荷转移态（charge transfer states）的自旋单三态的转化。我们针对这个中间过程建立模型进行了理论研究。首先，讨论了分子的热振动对于自旋态的弛豫过程，发现自旋单三态在存在分子热振动的时候会弛豫到单三态各占一半的末态，弛豫时间与温度成平方反比的关系。将这个弛豫过程引入到热活化延迟荧光中去，我们发现对于实验曲线拟合

的更好。其次，讨论了具有 Donor-Acceptor 结构的分子其给体受体连接桥的长度对于热活化延迟荧光的发光效率的影响。通过建立模型，我们计算了单三态能量差以及激子复合发光几率对于给体受体连接桥长度的依赖关系，讨论了发光效率随着连接桥的变化，发现连接桥具有一个最佳的长度，可以得到最高的发光效率。理论结果对于设计新的具有给-受体结构的热活化延迟荧光分子有借鉴意义。

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M-042

专题代号：M

矩形二维材料狄拉克锥形成的镜像对称分析

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摘要：石墨烯独特的狄拉克锥能带结构最初被认为与其六角晶格对称性有关。然而，具有矩形单胞的二维材料如一元的 6,6,12-石墨炔和二元的 t1/t2-SiC 等也相继被发现具有狄拉克锥能带结构。近年来我们提出了系列的“分组-耦合”机制解释各种二维材料的狄拉克锥能带结构成因[1-3]。本工作首次从对称性分析角度对二维材料狄拉克锥形成起源进行了研究。我们结合紧束缚方法和密度泛函理论计算，通过对原子排列和原子波函数的对称性分析，提出了“镜像对称的奇偶耦合”机制来解释 6,6,12-石墨炔狄拉克锥能带结构的形成机制。首先，单胞中的原子被分成分别具有镜像对称性的两组(G1 和 G2)，对每组内部的原子波函数进行组合，获得两组新的正交归一的完备基组，使得其中每个基矢具有确定的镜像宇称（奇宇称或偶宇称）。从而共获得四组正交归一基组：$G1^{+}$、$G2^{+}$、$G1^{-}$和 $G2^{-}$。然后对具有相同宇称（奇-奇和偶-偶）的组内和不同组间的基组先后进行分别耦合，最后对前面获得的奇偶不同的两组基组进行耦合，最终形成拉克锥能带结构（如图 1）。该机制能够解释具有镜像对称性的六角和矩形原胞的二维材料狄拉克锥能带结构的成因。本工作表明对称性分析对理解狄拉克锥形成具有重要意义，尤其是镜像对称性是比六角对称性更基本的对称性特征，可成为设计新型狄拉克锥材料的有力工具。

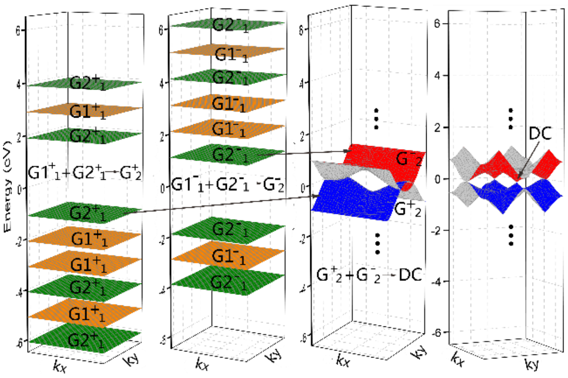

图 1 6,6,12-石墨炔狄拉克锥能带结构形成示意图：“镜像对称的奇偶耦合”机制

关键词：二维材料 狄拉克锥 紧束缚 密度泛函 对称性

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M-P001

专题代号：M

β-PtO_2：声子，热力学和弹性性质的第一性原理计算

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摘要：PtO_2 作为多用途催化剂广泛应用于光学、电化学和有机合成领域。目前的研究主要集中于实际应用，PtO_2 的晶格动力学及热力学性质都未曾研究。实验上确定了 PtO_2 的三种晶格结构，分别是：α-PtO_2（六角 CdI_2 结构）；β-PtO_2（正交 $CaCl_2$ 结构）；β′-PtO_2（四方 rutile 结构）。在常压下，β-PtO_2 最为稳定。全面了解 PtO_2 的基本性质是阐明 PtO_2 在光学和催化等领域应用中的作用和微观机理的先决条件。

中科院固体物理研究所杨勇研究员课题组采用第一性原理计算，系统地研究了常压下最稳定的 β-PtO_2 的结构、声子、热力学和弹性性质。利用声子谱和振动态密度研究了β-PtO_2 在不同压力下的晶格动力学和结构稳定性。随着压力的增加，β-PtO_2 光学模的振动频率增大，该结果与现有的实验数据比较符合。基于声子计算，我们研究了β-PtO_2 的比热容及压力对它的影响。比较了用不同计算方法得到的德拜

温度对压力的响应。并且通过 Voigt-Reuss-Hill 近似估计了弹性模量。我们发现，β-PtO_2 的体变模量随压力呈线性增加，然而剪切模量几乎与压力无关。进一步的研究表明，弹性刚度系数 C_{44}，C_{55} 和 C_{66} 在剪切模量的缓慢变化中起主要作用。

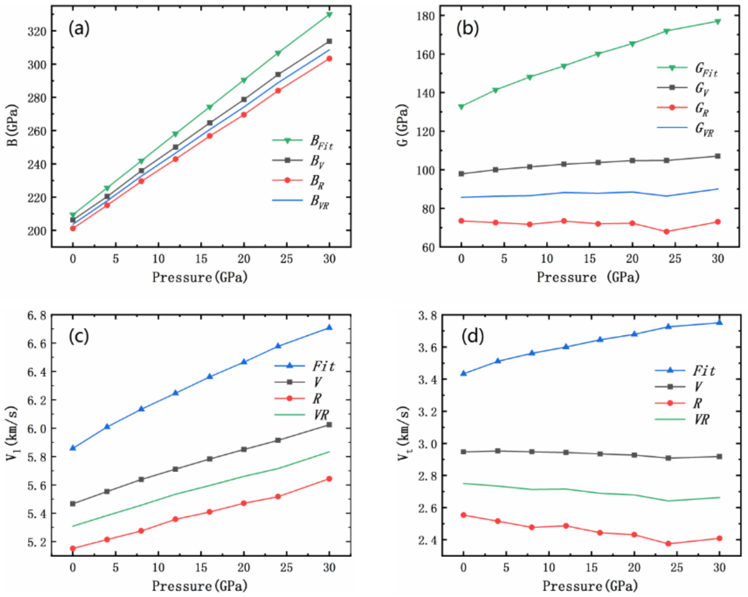

图 1 （a）体积模量，（b）剪切模量，（c）纵向声速和（d）横向声速随压力的变化

关键词：声子 热力学 弹性性质 β-PtO_2 第一性原理计算

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M-P002

专题代号：M

First-principles study on the mechanism of hydrogen adsorption and diffusion in $LaFeO_3$

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Abstract: Based on density functional theory, this paper studies the adsorption and the subsurface phase occupation by H on $LaFeO_3$ (010) surface and their corresponding transition states. As shown from the results, the best storage position of hydrogen are on the O top position of the $LaFeO_3$ (010) surface and the interstice near the oxygen of the bulk phase. In addition, the position of surface Fe atom can also store hydrogen, but H atom prefers to adsorb on O atom first. Whether the H atom is adsorbed on O or Fe atom, it is easy diffuse to the nearby more stable O atom. However, the diffusion between the Fe atoms is difficult to occur. The main diffusion path of the H atom from the surface to the bulk is the process of inward layer by layer around the O atom. With the fracture of the old H-O bond and the formation of the new H-O bond, the H is around O atom to constantly repeat the process of a hopping - rotational diffusion. H diffuses through the nearest neighbor position, which is more favorable than the direct diffusion.

Keywords: density functional theory; $LaFeO_3$; surface adsorption; bulk phase occupy; transition state

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M-P003

专题代号：M

InSe 纳米带提高析氢催化活性的第一原理研究

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摘要：在过去的几十年里，随着社会的发展和人口的增长，化石资源的消耗不断增加，导致能源资源的匮乏。同时，这导致二氧化碳排放量的增加，严重危害地球的生态环境。氢作为一种清洁能源载体，被认为是可再生能源技术中最重要的绿色能源候选之一。[1, 2]析氢反应(HER)制氢是一种环保的制氢方法，需要合适高效的催化剂来提供活性位点，以降低电能消耗。目前铂(Pt)等贵金属被认为是电化学 HER 上最稳定有效的催化剂，其过电位几乎为零。[3, 4]然而，自然资源的稀缺性和高成本限制了它们的实际应用。为了满足工业和实际的需要，需要新型高效、稳定、储量丰富的催化材料来促进水解制氢。为此，人们努力探索新的催化材料来取代铂。

课题组团队研究了一维 InSe 纳米带的边缘增强电催化性能。结果表明，锯齿状纳米带的电催化性

能与它们的边缘态有很强的关系，而这种关系可以通过平面空位进一步增强。在费米能级上，吸附的 H 原子的 s 轨道与 In 原子和 Se 原子的 p 轨道之间的相互作用增强了带隙态。这种相互作用导致在吸附氢的位置有显著的电子积累。电荷转移削弱了氢的吸附作用，降低了氢在演化过程中的能量。结果表明，局部成键促进了氢的演化活性。InSe 纳米带具有良好的催化性能，其高活性与吸附氢部位的电子积累有关。虽然没有缺陷的纳米带已经显示出令人满意的活性，但我们可以通过引入面内缺陷，在 In 或 Se 空位中进一步增强催化性能。从实验的角度来看，这个结果是非常有益的，因为在实验过程中几乎不可避免的会引入各种各样的缺陷。

关键词：二维半导体、纳米带、第一性原理

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M-P004

Effect of toxic ligands on O2 binding to heme andtheir toxicity mechanism†

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Yang Chen,a Yaqiang Ma*a and Yanan Tang *b

Heme, as the cofactor and active site of Hb, enables Hb to carry out the necessary function required for O2 management for life, that is, reversible O2 binding for transport. In this paper, the microscopic mechanism of heme-associated poisoning has been elucidated from the perspective of electronic interaction by performing first-principles calculations. The results show that the functional groups (–CHO, –COOH, –NO2, –NH2) and CN exhibit a stronger affinity for heme than O2 and are more likely to occupy the O2 binding site, which results in the loss of the ability of heme to carry O2. Moreover, the addition of functional groups, CO and CN to heme at the side site can cause a pronounced enhancement toward the O2 binding characteristics of heme, which prevents heme from releasing O2 to oxygen-consuming tissues as the blood circulates. The reversible O2 binding function of heme is disrupted by the presence of these toxic ligands in the heme binding pocket, which greatly affects O2 transport in the blood. The inability of tissues to obtain O2 leads to tissue hypoxia, which is the main cause of poisoning. Based on the energy, geometry and electronic properties, the hypoxia mechanism proposed by us coincides well with experiment, and the research has the potential to provide a theoreticalreference for the

relevant areas of bioscience.

M-P005

专题代号：M

Novel mechanical, magnetic and catalytic properties of 2D metallic transition-metal phosphides

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The fast development of two-dimensional transition-metal phosphides(TMPs) have received extensive interest due to their brilliant electrides and catalytic applications. Using first-principles calculation, we predict a new family of 2D tetragonal transition-metal phosphide (M2P, M=Fe, Co, Ni, Ru, Pd). We found all stable M2P are metallic with excellent extensibilities which display in low in-plane Young's modulus (89~167 N/M) and high ultimate tensile strength point (30%~45%). Interestingly, antiferromagnetic Fe2P and ferromagnetic Co2P with high Curie temperature (580K) exhibit novel magnetic properties. Furthermore, Ni2P display the best catalytic performance for its low overpotential which is benefit for multifunctional application in hydrogen evolution reaction(HER). Our work provides a new avenue in flexible eletride and electrocatalysis design.

M-P006

专题代号：M

蜂窝状单层中的超高可逆应变：从共价键到金属键

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摘要：我们关注到最近的一些关于二维铁弹体的理论研究，这些二维铁弹体理论上的可逆应变要比传统的铁弹体高出一个数量级。然而，它们的铁弹翻转在环境条件下可能难以实现，因为其铁弹翻转势垒太高，并且所需要的应力太大，在铁弹翻转的过程中可能会出现断裂。在这个工作中，我们探索了具有蜂窝状晶格(包括石墨烯、BN、锡烯等)的二维材料可能普遍存在的一种铁弹翻转路径，可以实现其扶手形方向和之字形方向的转换，其可逆应变达到了前所未有的 73.2%。

我们通过第一性原理计算发现，这种铁弹翻转路径在石墨烯和 BN 等共价体系中不起作用；然而，对于具有金属键的单层材料（如已经实验合成的锡烯、锡烷、单层 InBi 等），由于其铁弹翻转势垒和所需要的应力较小，并且在铁弹翻转过程中的最高能量/应力点仍在其弹性区，而有希望在环境条件下实现。这种应力应变行为的不同可以归结为共价键和金属键的不同特性：共价键具有定向性和刚性，而金属键具有韧性和延展性。像单层 InBi 这样的二元化合物甚至是面内铁电性和铁弹性耦合的多铁材料，并且由于其褶皱状结构，它还同时具有垂直铁电性。

我们进一步揭示了同族化合物的铁弹翻转势垒随金属性的增强呈线性下降的趋势。类似的行为可以推广到体态的闪锌矿或纤锌矿结构中，这两种结构可被视为褶皱状单层结构的多层叠加。

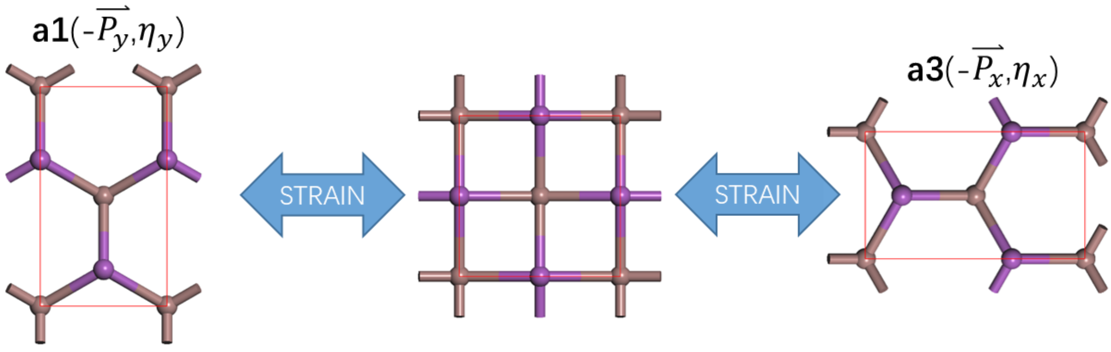

图 1 单层 InBi 的铁弹和铁电翻转动力学路径

关键词：铁弹性 铁电性 铁弹-铁电耦合 第一性原理计算

基金项目：国家自然科学基金项目（No. 21573084）

M-P007

专题代号：M

First-principles prediction of a new ground state for surface-oxidized phosphorene with remarkable piezoelectricity

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Abstract：In this paper, a new ground state (Pca21-PO) of surface-oxidized phosphorene is identified from a series of possible crystalline configurations. The crystalline structure of Pca21-PO is based on the previously proposed θ-P with further distortion. It is predicted to be more favorable than the previously proposed Pmn21-PO and confirmed to be dynamically stable. The calculated band structures show that Pca21-PO is an indirect band gap semiconductor with a gap of 0.607 eV and 1.396 eV based on DFT-PBE and HSE06 methods, respectively. It is a potential piezoelectric material with coefficients of −9.38 pm V^{-1}, 50.32 pm V^{-1}, 0.83 pm V^{-1} and –0.09 pm V^{-1} for d_{11}, d_{12}, d_{21} and d_{22}, respectively. These coefficients are comparable to those of group-IV monochalcogenides and more remarkable than that of the experimental MoS_2. In particular, Pca21-PO possesses piezoelectric effect in arbitrary direction in view of the absence of both inverse and mirror symmetries, which can be considered as a potential material for applications in nano-scale devices, such as sensors, actuators, electric field generators and any other applications requiring electrical and mechanical energy conversion.

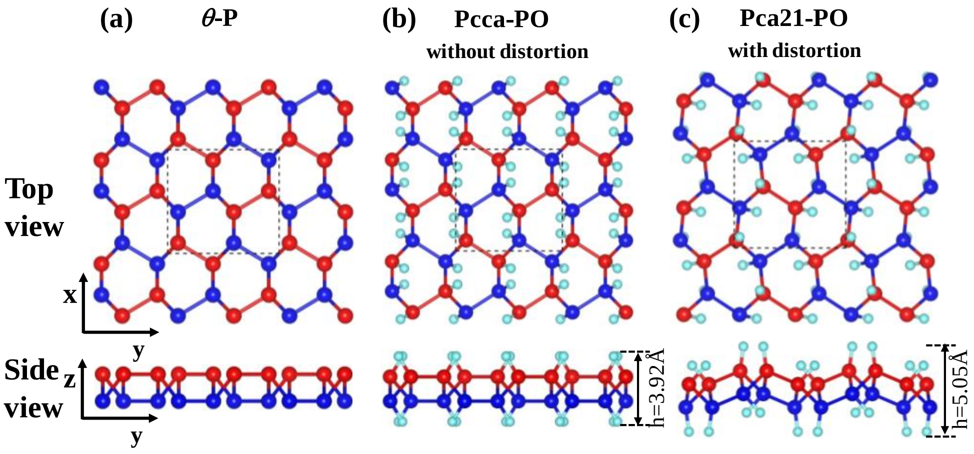

Figure 1. The crystalline structures of θ-P (a), Pcca-PO (b) and Pca21-PO (c).

Keywords: crystalline structure, surface-oxidized, piezoelectricity

【1】 Jiabin Li *et al.*, First-principles prediction of a new ground state for surface-oxidized phosphorene with remarkable piezoelectricity, *J. Phys. D: Appl. Phys.* 2019, 52 , 295301.

基金项目：国家自然科学基金项目（NOs. 11704319, 11647063, 11274262）

M-P008

专题代号：M

利用 DFT 探索 LaB6 声子输运特性及其对材料电热输运性质的影响

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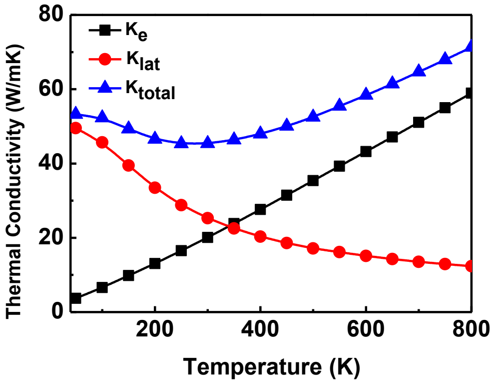
摘要：六硼化镧（LaB_6）由于具有低功函数、高硬度、高熔点、导电率高和使用寿命长等优点作为优良的热电子发射材料，因而被第一性原理研究。LaB_6 电子结构的计算表明，由于费米能级穿过导带且导带主要是 La 的 d 轨道电子的占据，所以 LaB_6 体现金属性行为，同时其电子性质与 La 的 d 轨道电子紧密相连。除以之外，通过分析计算 LaB_6 的声子谱和振动模式可知，局域的光学模主要是 B_6 八面体的贡献，La 原子不参与振动；B 原子的振动引起的 B_6 八面体畸变导致了光学模强烈的色散性行为，是体系晶格热导率的主要贡献，而扁平化的声学模对晶格热导率的贡献小，同时 La 的 d 轨道电子仅仅决定了体系的电子热导率，这在目前的探究中还未发现；在 350K—700K 温度范围内，与 B_6 八面体决定的晶格热导率相比，La 的 d 轨道电子决定的电子热导率对 LaB_6 总热导率的贡献更大，占据主导地位。基于得到的计算结果，我们提出了关于六硼化物（RB_6）热导机制的预测，并在实验中得到证实。

关键词：LaB_6；第一性原理计算；热导率；振动模式



LaB_6 热导率计算值的对比图

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M-P009

专题代号：M

Negative thermal expansion of Prussian blue analogues $ScCo(CN)_6$ and $TiCo(CN)_6$: First-principles study

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Prussian blue Analogues (PBAs) have been found to have many exotic properties[1]. However, the research on negative thermal expansion (NTE) of the compounds is rare and just beginning after the discovery of pronounced NTE in cubic ZrW_2O_8 by Slight's group[2]. In this poster, we present NTE of PBAs $ScCo(CN)_6$ and $TiCo(CN)_6$, which are calculated and analyzed using first principles density functional theory calculations combined with quasi-harmonic approximation. It is found that the two systems exhibit NTE caused by the low-frequency vibration modes. The modes mainly involve the vibrations of CN cyanide ligands, namely the lateral vibrations of the ligands. The low-frequency vibration modes have large values of negative grüneisen parameters. The calculated coefficients of thermal expansion are $-29.4\times10^{-6}K^{-1}$ at 144K for $ScCo(CN)_6$, and $-13.9\times10^{-6}K^{-1}$ at 96K for $TiCo(CN)_6$.

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基于二芳基乙烯分子的可逆分子光开关的合理设计

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摘要：单个二芳基乙烯分子的可逆光敏行为近年来引起了人们越来越多的关注，分子—电极耦合强度对实现双向电导开关起着至关重要的作用。在此，我们报告了基于光敏二芳基乙烯分子器件的第一性原理计算，采用非平衡格林函数结合密度泛函理论的方法计算了器件的电子输运特性和开关机理。研究结果表明，无论在器件中使用何种电极，两种异构体的导电率都存在很大的差异。开关行为本质上取决于分子本身的电子结构，这与之前的研究一致。重要的是该器件具有大的开关比，预计可达 10^3，且石墨烯电极器件中存在负微分电阻效应。这些发现对二乙烯类有机分子光开关的合理设计具有一定的指导意义。

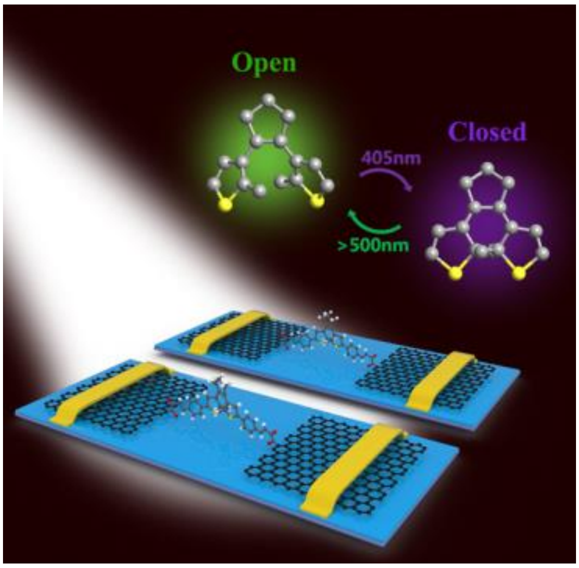

图 1 二芳基乙烯分子光开关器件示意图

关键词：二芳基乙烯 分子器件 分子光开关

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山东省重点研究开发项目(No. 2018GGX102008)

M-P011

专题代号：M

硼、镓、铟掺杂$Ca_{12}Al_{14}O_{33}$的电学性能第一性原理研究

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摘要：$Ca_{12}Al_{14}O_{33}$又简写为 C12A7，是钙铝相图中重要组成部分，近几年来，由于$Ca_{12}Al_{14}O_{33}$独特结构，作为立方晶体，每个单胞内有两个$Ca_{12}Al_{14}O_{33}$分子形成的由-O-Al-O-Ca-O-Al-六元环连接的 12 个球笼组成，在 12 个球笼中心处被两个游离的氧离子随机占据。因此具有天然纳米多孔结构、高比表面积、高离子电导率（离子电导率仅比氧化钇增强的氧化锆低一个数量级）、带隙宽等特点，具有广阔的应用前景，如作为用于燃烧挥发性有机化合物的新型高效催化剂、固体离子电解质、透明导电氧化物等引起了研究人员的广泛研究兴趣。已有大量实验探究了$Ca_{12}Al_{14}O_{33}$在不同掺杂情况下的导电率变化以及热力学稳定性，而关于其导电机理却知之甚少。为了探究不同阳离子掺杂$Ca_{12}Al_{14}O_{33}$对扩散势垒的影响，我们课题组将同一主族元素硼、镓以及铟掺杂到$Ca_{12}Al_{14}O_{33}$中的 Al1、Al2 两种位置，采用 Material Studio 软件建立掺杂模型，采用 VASP 软件包进行系统的晶格结构和电学基本性能计算的基础上，采用基于密度泛函理论的第一性原理方法，分别通过电荷密度分布以及电子结构，结合能带理论探讨离子电导率变化的原因，采用 c-NEB 方法讨论了框架外氧离子在不同掺杂模型中扩散势垒、路径变化。

关键字：掺杂 $Ca_{12}Al_{14}O_{33}$ 氧扩散 能带理论 第一性原理计算 电子结构

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基金项目：广西科技计划项目 (NO. 2018GXNSFAA050013) 。

M-P012

专题代号：M

高压下氨-氢化合物新奇的结构

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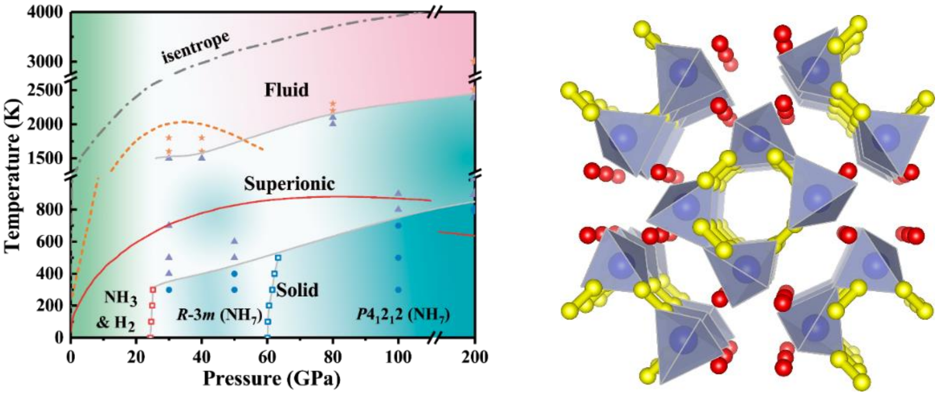
摘要：氨和氢是天王星和海王星等行星内核的重要组成成分[1]，它们是否会在行星内核条件下发生化学反应备受关注。澄清该问题的关键是确定二者能否在高温高压下形成稳定的化合物。本项目利用CALYPSO方法[2-4]确定了氨-氢化合物的高压相结构，并研究了其相应的电子性质和化学键演变行为。计算数据显示NH_3和H_2在高压下可以发生化学反应，生成两个具有新奇元素配比的离子相NH_7。低压相结构具有菱方对称性，部分H_2分子分解为质子和氢负离子，形成氢桥键和双氢键。在更高的压力下，NH_3吸引质子的能力增强，形成包含NH_4^+结构单元的四方相。随着温度的升高，离子相结构转变为新奇的超离子态，兼备固态相和液态相的双重特征。当前的研究丰富了行星内部物质高压行为的认知，为储氢材料的创新设计和性能优化提供了新思路。



图一 氨-氢化合物 NH_7 的温度-压力相图及 $P4_12_12$ 相晶体结构

关键词：结构预测，第一性原理，晶体结构，高压，氢键，超离子相

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基金项目：国家自然科学基金项目（NO. 11622432, 11534003）
国家重点研发计划项目（NO. 2016YFB0201200）

M-P013

半氢化石墨烯与 Bi_2Se_3 异质结的第一性原理研究

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基于密度泛函理论的第一性原理，我们研究了铁磁半导体半氢化石墨烯（SG）对拓扑绝缘体 Bi_2Se_3 薄膜电子性质的影响。根据计算结果，由 C 原子孤立电子对所形成的磁矩在异质结界面产生的磁近邻效应破坏了体系的时间反演对称性，进而在界面态的相互作用下分别打开了 3QL 和 5QL Bi_2Se_3 薄膜的第一 QL 的表面态，形成了一个约为 40meV 和 150meV 的巨大磁致带隙。相对于 Bi_2Se_3/MnSe 异质结结构的 56meV[1]，我们的研究结果很好地解决了目前磁性原子诱导拓扑绝缘体表面态带隙较小的问题，这为更好地实现拓扑磁电效应[2]提供了很好模型系统。同时，由于 AB 型异质结的构建导致空间反演对称性的打破，3QL 和 5QL 的 Bi_2Se_3 薄膜体系均出现了明显的 Rashba 自旋劈裂现象。通过对孤立 C 原子进行 H 饱和的研究发现，Rashba 自旋劈裂现象[3]对于体系磁性的有无具有明显的依赖性，即 Rashba 自旋劈裂在磁场的作用下会有明显的增强，这一现象为磁场调控 Rashba 劈裂提供了新的途径，并且也显著地拓宽了自旋电子器件的应用范围。此外，本文采用非磁性原子构建的异质结为铁磁--拓扑绝缘体异质结的研究提供了新的思路和方法，并为在研究铁磁拓扑绝缘体异质结的性质和自旋电子器件的应用上提供了更多可能性。

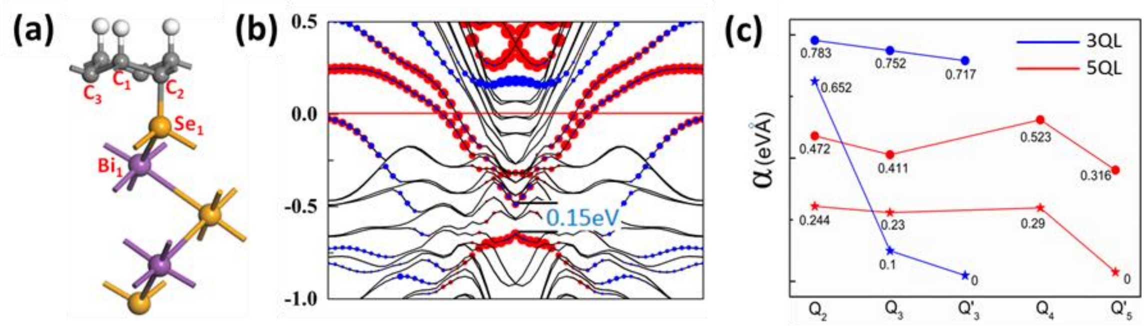

Fig. 1(a) $(\sqrt{3}\times\sqrt{3})$SG/$(1\times1)Bi_2Se_3$ 异质结结构示意图。(b) SG/5QL Bi_2Se_3 的能带图，其中黑色线代表的是总能带，红色点线和蓝色点线分别代表的是第一 QL 和 SG 的在总能带上的投影。(c) SG/3QL Bi_2Se_3 和 SG/5QL Bi_2Se_3 能带劈裂的 Rashba 参数 α_R(其中点线表示为磁性异质结，星线表示为非磁性异质结)

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M-P014

专题代号：M

体态和二维卤化银、卤化亚铜中的相变以及多铁性

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摘要：诸如 AgBr、AgI 这样的卤化银是众所周知的用于照相和光化学的感光材料，在室温条件下卤化银和卤化亚铜倾向于形成闪锌矿型结构，根据菲利普斯量表，它们的离子性接近 0.7，略低于临界值 0.785，标志着“共价”和“离子”系统之间的理想边界。在这项工作中，我们首次报告了环境条件下卤化银和卤化亚铜可能的铁电性和的铁弹性。

我们通过第一性原理计算证明：卤化银和卤化亚铜在非极化岩盐相和极化闪锌矿相之间具有相对较低的转换势垒。这种相对较低的转换势垒使得这两种单卤化物具有新颖的机械和电子性质，即在环境条件下拥有较高极化和较低切换势垒的铁电性和铁弹型耦合。一些卤化物甚至具有与诸如硅等主流半导体非常相似的晶格常数和结构，从而能够在硅上进行外延生长。并且我们通过 CALYPSO 结构搜索，发现最稳定的单层卤化物的二维多晶型具有接近甚至大于他们体态对应物的内聚能，这在岩盐或闪锌矿型半导体结构中比较少见。我们预测了闪锌矿相和层状体态相之间比较低的转换势垒，并且一些二维单层卤化物具有耦合铁电性/铁弹性的多铁性，从而赋予它们可以用于高效数据读取和写入的高密度集成存储器件的应用潜力。它们的表面覆盖有卤化物提供了抗氧化性。它们层状结构较低剥离能表明通过实验剥离的方法得到这些 2D 多晶型的可能性很高。

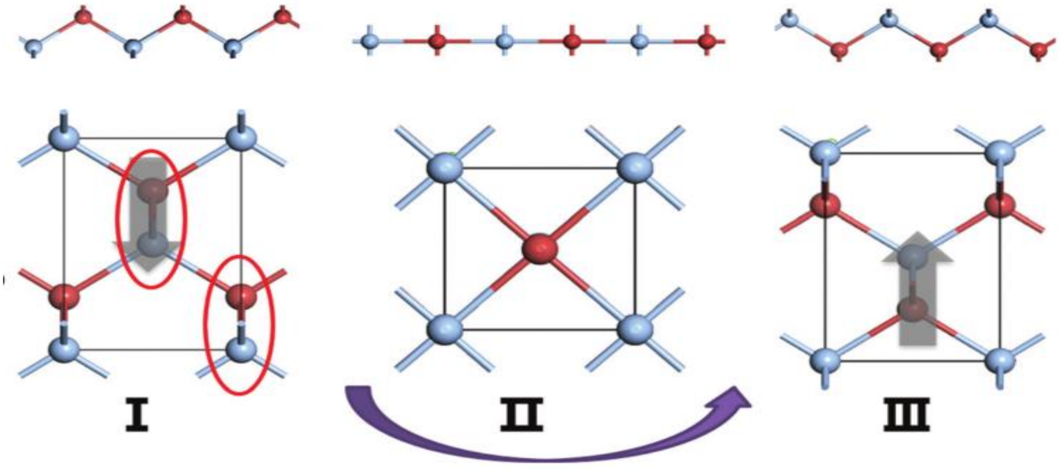

图 1 闪锌矿型 AgI 的铁电翻转路径

关键词：第一性原理计算 相变 铁弹性 铁电性 铁弹-铁电耦合

基金项目：国家自然科学基金项目（No. 21573084）

M-P015

专题代号：M

压力诱导的 LiP$_{15}$ 的维度变化和超导特性

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摘要：近年来，石墨烯、过渡金属硫化物、氮化硼以及黑磷等层状材料，因其具有卓越的电子、热学、光学和力学性能受到人们的广泛关注。通过控制层数、施加外场和化学掺杂可以调控这些材料的电子结构，诱导出新奇的物理性质，如超导特性。我们可以利用层状材料作为前驱体，通过化学溶剂法、物理剥离法等方法来制备单层或少层二维材料。寻找新型vdW（范德瓦尔斯）层状材料并探索其物理性质是当今凝聚态物理领域及交叉学科领域研究热点。

最近，我们研究了压力诱导的vdW材料LiP$_{15}$在低于10 GPa压力下的结构相变和电子特性。半导体P-1相在相对低的压力（约2 GPa）下转变成新预测的金属$C2/m$相。结构上，磷原子从准一维管状结构转变为具有褶皱的二维结构。有趣的是，P-1相的磷子结构与红磷(red-IV)结构相似，而新发现的$C2/m$相的磷子晶格与空位嵌入的蓝磷结构相似。金属相$C2/m$表现出良好的超导特性，在2 GPa下超导转变温度T_c为2.3K，并且T_c随着压力的升高逐渐增大，在10 GPa压力下，T_c为9.6K。进一步，我们通过去除P-1和$C2/m$相中的锂原子，成功获得了两个热动力学稳定的新的磷同素异形体。环境压力下使用不同的范德瓦尔斯力的修正，两者的能量都非常接近于黑磷的能量。这项工作不但可以帮助我们加深对二维材料的前驱体——层状材料的理解，而且丰富了多磷化物衍生的磷同素异形体结构。

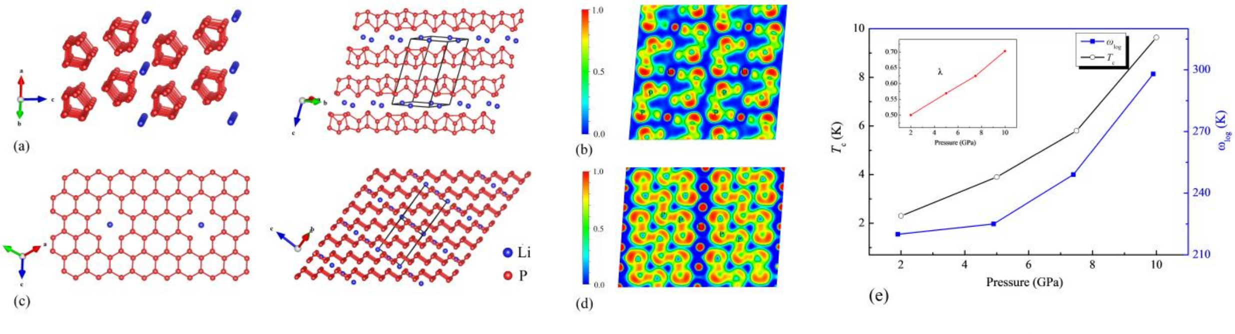

图 1　P-1 和 $C2/m$ 结构图(a)和(e)；ELF 图(b)和(d)；$C2/m$ 结构的 T_c、ω_{log}和λ随压力变化曲线

关键词：晶体结构预测 结构相变 层状材料 超导 磷同素异形体

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M-P016

专题代号：M

Layzer 模型下压缩对 Rayleigh-Taylor 和 Richtmyer-Meshkov 不稳定性的影响

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摘要：在改进的 Layzer 模型下，研究了压缩对 Rayleigh-Taylor (RT)和 Richtmyer-Meshkov (RM)不稳定性的影响。从绝热方程$\frac{p}{\rho^{\gamma}} = const$可以看到，绝热系数 γ 可以作为一个表示不易压缩性的参量。为了能反映实际的不稳定性发展过程中界面处的压强、界面两侧密度的随界面运动速度的动态变化，我们还引入一个动态变化的驻点压强$P = p \pm \frac{1}{2}\rho U^2$，它可以将流体的实际密度与界面速度联系起来。借此，在 Layzer 模型的框架下，可以推导出关于可压缩流体的 RT 及 RM 不稳定性随时间发展的方程组，从而可以人为给静压强 p、界面两侧的静密度 ρ_{u0} 和 ρ_{l0}、界面两侧的绝热系数 γ_u 和 γ_l 赋值，这样就可以定量研究界面的振幅、速度和曲率半径随时间的演化。研究发现，对于 RT 不稳定性，界面上侧的绝热系数 γ_u 和密度有使 bubble 的振幅和速率增大，以及使早期阶段的曲率半径减小的效应；界面下侧的绝热系数 γ_l 和密度则有使振幅和速率降低，以及使早期的曲率半径增大的效应。然而，可压缩性并不影响 RT 不稳定性末态（bubble 速率不再随时间变化）的曲率半径。此外，当存在压缩性，我们发现可能会有上侧静态密度大于下侧却不能发生持续的 RT 不稳定性，或者上侧静态密度小于下侧但仍可发生持续的 RT 不稳定性的密度取值区间，这与不考虑压缩性的情况有明显的不同。对于 RM 不稳定性，上侧的绝热系数 γ_u 和密度有使振幅以及速率减小，以及使早期的曲率半径增大的效应。而下侧的绝热系数 γ_l 和密度则有使振幅及速率增大，以及使早期的曲率半径减小的效应。然而，对于 RM 不稳定性，当时间稍微增大时，可压缩情况下的曲率半径趋于与不可压缩的情况相同。

关键词：Rayleigh-Taylor 不稳定性　Richtmyer-Meshkov 不稳定性　Layzer 模型　压缩性

M-P017

专题代号：M

Biaxial strain induced band transition and valley–spin coupling in the ferromagnetic semiconducting WSe_2/1T-$FeCl_2$ heterostructure

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The structural and electronic properties of the WSe_2/1T-$FeCl_2$ heterostructure have been investigated by density functional theory and Berry curvature calculations. The heterostructure is a magnetic semiconductor with type-II band alignment (0.35 eV band gap) and a magnetic moment of 3.872 μ_B per unit cell, and it has a high Curie temperature of 816 K by calculating the different magnetic configurations. In addition, the two layers of the heterostructure couple with each other by van der Waals force based on the Bader charge analysis. Biaxial strain causes a transition of the band alignment from type-II to type-I, and it also leads to a significant change in the work function. Under compression strain of -2% to -8%, the electronic band of the heterostructure shows valley-contrasting character and valley-spin coupling, like monolayer WSe_2. The Berry curvature and spin splitting are opposite at the K and K′ valleys, so the valleys and spins are simultaneously locked and polarized, and the valley Hall effect and spin Hall effect simultaneously occur.

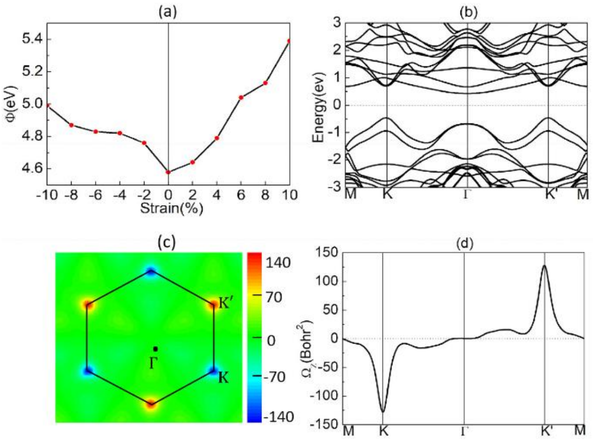

Fig.1 (a) Variation of the work function as a function of biaxial strain. (b) Band structure calculated by the MLWFs, (c) contour map of the Berry curvature in the 2D Brillouin zone, and (d) Berry curvature of the WSe_2/$FeCl_2$ heterostructure at compression strain of −6%.

Keywords: Heterostructure, Valley, Band alignment, Berry curvature

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M-P018

专题代号：M

Long wavelength acoustic modes driven negative thermal expansion in rhombohedral Zn_2GeO_4: A first-principles investigation

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Abstract: Zn_2GeO_4 was reported to exhibit negative thermal expansion (NTE) below room temperature in experiment. However, the underlying mechanism of NTE has not been reported. In this work, we investigate the NTE in rhombohedral Zn_2GeO_4 using first-principles methods combined with quasi-harmonic approximation. Calculations show that the system exhibits NTE below ~200 K and the calculated coefficients of NTE is in reasonable agreement with experiment. Detailed analysis of the phonon modes reveals that the low-frequency acoustic modes near the center (Γ point) and boundary of the first Brillouin zone, dominated by the collective movement of the Zn and Ge atoms along with their neighboring oxygens, mainly contribute to the NTE of the Zn_2GeO_4, which is in contrast to the conventional NTE mechanisms for the open-framework structures of oxides, where the phonon modes, such as transverse vibration and libration of bridge oxygens and rotations of the rigid-unit modes, play key roles in the NTE of the materials. Our results give a new understanding of NTE mechanisms for the more flexible framework oxide materials.

Keywords: first-principles calculations, Zn_2GeO_4, NTE mechanisms, acoustic modes

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基金项目：国家自然科学基金项目（No. 11874328; No. 11574276）

M-P019

专题代号：M

CrB_2单层的第一性原理研究：一种新的二维铁磁性半导体

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摘要：近年来，二维铁磁半导体因其可以利用自旋自由度来提高半导体器件功能而成为理想的半导体材料。本文通过基于粒子群优化算法的晶体结构搜索方法（CALYPSO）和第一原理一系列计算，预测了一种迄今未知的二维 CrB_2 (P6mmm)单分子层，它是一种本征铁磁半导体材料，磁矩为 1.5μB，间接带隙大小为 0.55 eV。电子从 Cr 原子转移到硼层这不仅有效的稳定了 CrB2 网络而且导致了 Cr 和 B 原子之间的强相互作用，同时计算表明 CrB2 单层具有较强的动力学和热力学稳定性，因此其具有较强的实验可合成性。利用经典海森堡哈密顿量的统计蒙特卡罗模拟方法，对磁性质的热依赖性和磁跃迁的居里温度进行了评价，居里温度结果为 134~201K。我们的研究拓宽了现有的二维材料家族，在纳米电子学中具有广阔的应用前景。

关键词：二维材料、铁磁、半导体、自旋电子学

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M-P020

专题代号：M

Strain effect on magnetic transition and magnetic anisotropy energy in 2D two coordinated 5d transition metal

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Quantum information and spintronics devices, based on searching and manipulating magnetism, open up new questions in the studies of two dimensional materials. Using first-principle calculations, here we design a novel type of 2D metal organic frameworks (MOFs), which is composed of (1, 3, 5)-benzenetricarbonitrile (TCB) molecules linked with 5d transition metals (i.e., Hf, Ta, W, Re, Os, Ir), namely TCB-TM. Owing to their low coordinated, half-filled 5d electronic configuration, and suitable crystal field, robust ferromagnetism semiconductor with 63 meV bandgap, large magnetic anisotropy energy (19 meV/atom) and room temperature Curie temperatures (613 K) are found in TCB-Re monolayers. Remarkably, with the help of biaxial strain, a reversible magnetic transitions between ferromagnetic and antiferromagnetic have been found and the magnetic anisotropy energy is even increased up to 120 meV/atom. Meanwhile, large magnetic moment and room Curie temperature have been well preserved. To provide more insights into generally spin control mechanism, strain induced energy level regulating, bond reduction, orbital hybridization, magnetic interaction, and exchange coupling parameter have also been discussed. Our theoretical results point out that strain engineering is an effective method to manipulating spin and enhance the magnetic anisotropy energy to TCB-TM monolayer, which pave the way for experimental design of spin and magnetic storage devices.

Keywords: 5d transition metal; magnetic transition; magnetic anisotropy; strain

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M-P021

专题代号：M

Few-layer β-SnSe with Strong Visible Light Absorbance and Ultrahigh Carrier Mobility

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Abstract：The solar cell which uses the photovoltaic effect to convert solar energy into electricity directly has aroused widespread attention. Compared with traditional bulk materials, two-dimensional (2D) materials can exhibit exotic optoelectronic properties and especially provide large photoreactive contact areas, making them more attractive for designing novel optoelectronic devices. In this work, we use the first-principles methods based on density functional theory to study the electronic and optical properties of few-layer β-SnSe. It is found that the one-layer, two-layer and three-layer β-SnSe are semiconducting with direct band gaps of 1.38 eV, 1.20 eV and 1.05 eV, respectively, which fall within the optimum band gap for solar cells. The optical absorbance and upper limit of the energy conversion efficiency can reache values as high as 56% and 15.4%, respectively, for three-layer β-SnSe, which is comparable to the current efficiency records. Furthermore, the few-layer β-SnSe has very high carrier mobility, reaching 10^7 $cm^2V^{-1}s^{-1}$ for the three-layer β-SnSe . The strong visible light absorption and high carrier mobility of few-layer β-SnSe provide promising opportunities for applications in solar cells.

keywords：few-layer, strong visible light absorbance, ultrahigh carrier mobility, solar cells

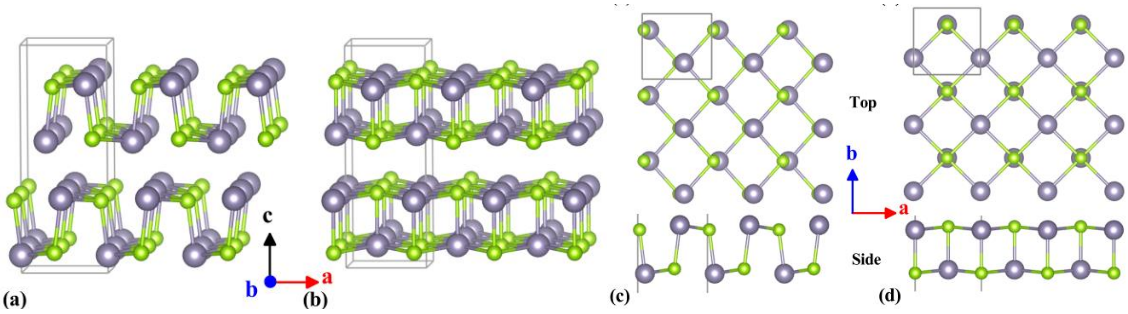

Fig. 1 Crystal structures of bulk (a) α-SnSe of the Pnma space group (#62) and (b) β-SnSe of the Cmcm space group (#63), with the top and side views of one-layer (c) α-SnSe and (d) β-SnSe. The cuboid frames show the orthorhombic unit cells. Gray and green balls represent Sn and Se atoms, respectively.

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M-P022

专题代号：M

二维磁性材料设计

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摘要：二维磁性材料，如 CrI_3 或者 $Cr_2Ge_2Te_6$ 的成功制备，使其在自旋电子器件、信息存贮等方面的重要应用日益成为现实。寻找性能卓越的二维磁性材料的研究风起云涌，成果丰硕。其中重要的理论进展之一是利用晶体数据库，基于已有的层状三维磁性材料，通过高通量筛选的方法，预测 56 个二维磁性材料可以从母体中剥离，例如已合成的 CrI_3 或者 $Cr_2Ge_2Te_6$。然而，对于晶体数据库中缺失的、或者原本就不存在母体三维磁性材料的情况，高通量筛选的方法将失效。针对这种情况，我们发展了基于进化算法的二维磁性材料搜索算法，不仅可以高效重复高通量筛选方法的结果，而且可以寻找无层状母体的新颖二维磁性材料。应用该方法于二维 CrI_3 体系，计算结果表明该体系的基态结构为铁磁 $P31m$-CrI_3，与实验结果一致。应用该方法于非传统磁性的二维 B 体系，预测磁性硼烯，发现了稳定的反铁磁半导体 $P6/mmm$-B_{19}。$P6/mmm$-B_{19} 不仅具有可调磁性，在少量电子掺杂的情况下发生反铁磁半导体-铁磁半金属的相变，同时还具有少见的面外负泊松特性，是独特的多功能材料。应用该方法于三维母体非磁、非层状的二维 CrB_4 体系，发现了稳定的铁磁金属 Cm-CrB_4。磁性材料搜索算法系统的研究体系的磁相图，拓宽了二维磁性材料研究的范围，丰富了二维磁性材料的种类，对于指导实验研究和自旋电子器件应用的实现具有重要意义。

(a)

图 1 (a) 二维磁性材料搜索方法结构产生示意图。

关键词：二维磁性材料搜索算法，二维磁性材料，第一性原理，电子性质

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M-P023

专题代号：M

Intrinsic Half-Metallicity in 2D Ternary Chalcogenides with High Critical Temperature and Controllable Magnetization Direction

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Searching for 2D ferromagnetic materials with a high critical temperature, large spin polarization, and controllable magnetization direction is a key challenge for their broad applications in spintronics. Here, through a systematic study on a series of 2D ternary chalcogenides with first-principles calculations, it is demonstrated that a family of 2D $CoGa_2X_4$ (X = S, Se, or Te) are half-metallic ferromagnets, and they exhibit high critical temperature, fully polarized spin state, and strain-dependent magnetization direction simultaneously. Following the Goodenough–Kanamori rules, the half-metallic ferromagnetism of $CoGa_2X_4$ family is caused by superexchange interaction mediated by Co–X–Co bonds. The half-metal gaps are large enough (>0.5 eV) to ensure that the half-metallicity is stable against the spin flipping at room temperature. Magnetocrystalline anisotropy energy calculations indicate that $CoGa_2X_4$ favor easy plane magnetization. Under achievable biaxial tensile strain (2–6%), the magnetization directions of $CoGa_2X_4$ can change from in-plane to out-of-plane, providing a route to control the efficiency of spin injection/detection. Further, the critical temperatures Tc of ferromagnetic phase transition for $CoGa_2X_4$ are close to room temperature. Belonging to the big family of layered AB_2X_4 compounds, the proposed $CoGa_2X_4$ systems will enrich the available 2D candidates and their heterojunctions for various applications.

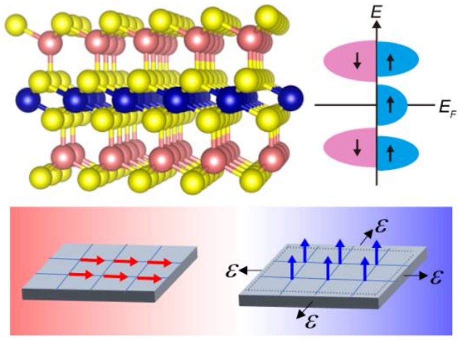

Fig. 1 The schematic diagrams of structure, band structure, strain tunable magnetism in $CoGa_2X_4$

Keywords: half-metallicity, ternary chalcogenides, spintronics, first-principles calculations

Funding: China Postdoctoral Science Foundation (No. 2018M631458)

Reference: S Zhang, R Xu, W Duan and X Zou. Adv. Funct. Mater. 2019, 29 (14), 1808380.

M-P024

专题代号：M

Saddle-point Excitons and Their Extraordinary Light Absorption in Two-Dimensional β-phase Group-IV Monochalcogenides

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Abstract

In two-dimensional (2D) materials, saddle-points in the electronic structure give rise to diverging density of states, which leads to intriguing physical phenomena useful for applications, including magnetism, superconductivity, charge density wave, as well as enhanced optical absorption. Using first-principles calculations, we show monolayer β-phase of group-IV monochalcogenides (MX, M = Ge or Sn; X = S or Se) are a new class of 2D materials that possess saddle-points in both the lowest conduction band and the highest valence band as well as in the joint density of states. Due to the existence of saddle-points, a remarkable absorption peak within the fundamental gap is found in these materials when the light polarization is along the armchair (y) direction. The properties of saddle-point excitons can be effectively tuned by both the strain and thickness of these materials. Importantly, the strong optical absorbance induced by saddle-point exciton absorptions and the appropriate band gap give ideal power conversion efficiencies as large as 1.11% for monolayer β-SnSe, significantly higher than reported high-performance ultrathin solar cells using transition metal dichalcogenides. These results not only open new avenues for exploring novel many-body physics, but also suggest β-phase MXs could be promising candidates for future optoelectronic devices.

Keywords：two-dimensional materials, group-IV monochalcogenides, saddle-point excitons, solar cells, first-principles calculations

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M-P025

专题代号：M

多尺度纯排斥相互作用系统动力学特性研究

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摘要：多尺度相互作用粒子系统，尤其是具有竞争排斥和吸引相互作用粒子系统[1]，由于存在着丰富的相和相变[2]，所以一直是大家关注的焦点。最近，有人指出：多尺度纯排斥相互作用系统也会出现类似于竞争排斥和吸引相互作用系统的有序现象[3]。本文利用郎之万分子动力学，系统考察弱无序钉扎衬底上几种二维双排斥（粒子间具有长程库仑+中长程磁偶极子、中长程磁偶极子+短程屏蔽库仑、短程 Lennard-Jones +短程屏蔽库仑等纯排斥相互作用）系统的动力学特性，特别是脱钉特性。研究发现：短

程且力程相近的双排斥相互作用系统在脱钉点以上更容易出现有序运动，且比单尺度纯排斥相互作用系统有序明显。这对于揭示生物系统的活性起源提供有价值参考。

关键词： 多尺度 排斥相互作用 动力学 有序

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M-P026

专题代号：M

高压下新型 He-N 组分

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摘要：近年来，新型含能材料在航天、军事等领域有着重要的应用价值，可用作炸药、导弹和运载火箭的推进剂等，设计与合成新型高能量密度材料是凝聚态物理和材料科学的研究热点之一。其中，富氮化合物以高密度，高反应速度，高安全性以及较低合成压力等优势而备受关注。与传统的含能材料不同，富氮类化合物的结构决定了其高能量密度特性。

N_2 和 He 在环境条件下由于其化学惰性不发生相互作用，但高压能突破这种限制。目前实验上已知的仅有 $He(N_2)_{11}$ 范德华晶体[1]。基于晶体结构预测软件 USPEX 结合密度泛函理论计算，研究了在 0-100GPa 压力范围内的 He-N 化合物，系统探索高压下可能的亚稳 He-N 组分[2]。研究发现，在某些压力区间有特定组分具有较好的热力学稳定性和动力学稳定性。计算表明 HeN_{10} 和 HeN_{22} 两种结构可以卸压到常压，其能量密度分别为 10.45 kJ/g 和 10.72 kJ/g，是潜在的高能量密度材料。它们的成功预测揭示了高压下 He-N 体系结构多样性，加深了人们对氮化物的理解，为高压实验合成新型高能量密度材料提供了理论指导。

关键词：高能量密度材料，USPEX，密度泛函理论，氦氮化合物

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M-P027

专题代号：M

(Ru+N)共掺杂对锐钛矿 TiO_2 光催化性质的优化理论研究

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摘要：无毒稳定的 TiO_2 是一种非常重要的光催化剂，尤其是在光分解水制氢方面。然而实际的应用常常受制于其过大的带隙(3.2 eV)只吸收紫外光，为此基于“减小能带工程”的思想，通过金属与非金属共掺杂来提高锐钛矿 TiO_2 的可见光吸收和光催化性质是目前较为有效实用的方法。利用密度泛函理论，我们系统的研究了单原子 Ru 和 N 在单掺杂和共掺杂 TiO_2(101)表面的掺杂位置和总能、几何结构、电子结构和光催化性质。计算发现，在 Ru、N 单掺 TiO_2(101)表面的系统中，由于杂质能级在禁带中形成了局域的未占据态，可能成为光生载流子的复合中心，降低其光催化效率。然而当(Ru+N)共掺杂 TiO_2(101)表面时，由于阴阳离子引入补偿施主和受主对，在费米能级附近产生可以作为电子跃迁的跳板的中间带，从而促进电子和空穴的分离，使光学性质得到提高。此外，禁带产生的中间带会导致光子激发能量降低和光吸收能力提高，使得锐钛矿 TiO_2 的吸光范围发生红移，将吸收光谱范围扩大至可见光范围。进一步的，我们分析了对不同掺杂模型对光解水性质的影响，通过比较水的还原与氧化势差发现，共掺杂体系的还原氧化电势有利于光解水的有效进行。另外从动力学角度对(Ru+N)共掺杂 TiO_2(101)面的析氢反应和性能进行研究，发现共掺杂体系的 HER 反应速率高于未掺杂和单掺杂的 TiO_2(101)面。本文结果表明，(Ru+N)共掺杂 TiO_2(101)面可以有效的提高材料的光催化性质，有利于光分解水制氢。

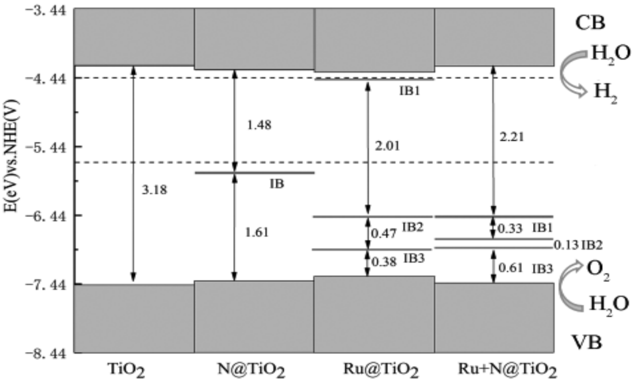

图 1 不同掺杂体系与水分解的还原氧化电位对比

关键词：锐钛矿 TiO_2 共掺杂 光催化 密度泛函理论

基金项目：国家自然科学基金项目（N0.21431003）

M-P028

专题代号：M

直接 Z-Scheme $BC_3/C_3N(BC_6N)$ 异质结光催化水分解的理论研究

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摘要：最近，在光催化水分解领域有着优异性质的二维类石墨烯材料（如 g-C_3N_4、C_2N）引起了广泛的研究兴趣，不同于石墨烯的是它们有着较宽的带隙。对于可用于水分解的光催化剂，首先要满足合适的带隙值，以能够吸收大部分可见光；其次，它们的导带底（CBM）的位置要高于水的还原电位，价带顶（VBM）的位置要低于水的氧化电位，这样才能进行光催化水分解反应。除此之外，光催化剂的低成本、无毒、在水溶液中高稳定性也是重要的条件。通过第一性原理方法，我们计算并比较了三种新的二维类石墨烯材料（BC_3、C_3N 和 BC_6N），它们有着石墨烯一样的六方平面结构。BC_3 和 C_3N 均是间接带隙半导体，带隙值分别为 1.83 eV 和 1.04 eV；而 BC_6N 是直接带隙半导体，带隙值为 1.83 eV，其中 BC_3 和 BC_6N 适合用于光催化水分解反应。由于在单一的半导体中光生载流子复合率较高，限制了其光催化效率，所以我们构建了两种“Z-scheme”异质结，分别为 BC_3/C_3N 和 BC_3/BC_6N。在这两类异质结中，光辐照下各个组成半导体分别产生光生载流子，通过接触界面发生了“异类半导体”间光生电子和光生空穴的有效复合，从而达到界面平衡。结果留在 C_3N 和 BC_6N 侧的光生电子主导析氢反应，而留在 BC_3 侧的光生空穴主导析氧反应。相比较而言，BC_3/BC_6N 异质结对可见光的吸收更好。该类“Z-scheme”异质结设计有利于光生电子和空穴的有效空间分离，提高了光催化水分解的效率。这项工作为非金属水分解光催化剂的理论设计和实验制备提供了一种有效的方法。

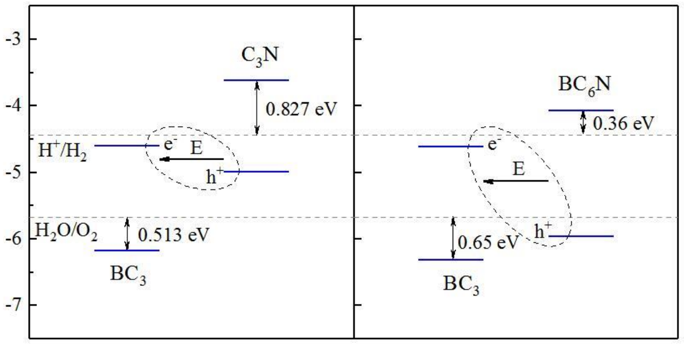

图 1 $BC_3/C_3N(BC_6N)$ Z-scheme 异质结的光催化水分解示意图

关键词：水分解反应 光催化剂 Z-scheme 异质结 第一性原理 二维类石墨烯材料

基金项目：国家自然科学基金项目（N0. 21431003）

M-P029

专题代号：O

新型层状 $K_{0.8}Ni_{0.4}T_{1.6}O_4$ 纳米片：合成、微观结构和对 MB 的光催化降解

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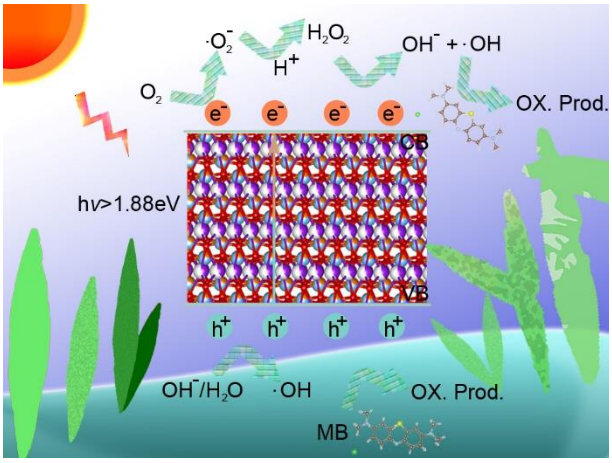
摘要：二氧化钛基的材料被广泛研究应用在各式各样的领域包括敏化太阳能电池、气体传感器,光催化合成及光电,电变色,光化学,燃料电池,生物抗菌等。在过去几年里,许多的方法被应用于提高二氧化钛光催化活性的金属硫化物形成异质结负载金属或金属氧化物纳米粒子,或掺杂非金属和金属原子。在染整过程中，每年有近 $2×10^5$ 吨工业染料流失到废水中，对我国水资源造成严重污染。迫在眉睫的是研究新型高效的染料降解材料。过渡金属掺杂 TiO_2 用来光催化降解水中有机污染物也是近年来的研究热点。

近年来，我们先后采用简单的一步水热法合成了 $Na_{0.9}Mg_{0.45}Ti_{3.55}O_8$、$Na_2Fe_2Ti_6O_{16}$ 和 $K_{1.46}Fe_{0.8}Ti_{7.2}O_{16}$。现在,$K_{0.8}Ni_{0.4}Ti_{1.6}O_4$ (KNTO)也通过这种方式制备获得[1, 2]。然而,这种材料于 1980 年首次由固相方法合成，并没有深入彻底的内在特征表征和物理化学性能测试。作为单晶，KNTO 具有竹叶状般的形貌。除此之外， KNTO 与 $Na_2Fe_2Ti_6O_{16}$ 和 $K_{1.46}Fe_{0.8}Ti_{7.2}O_{16}$ 一样享有双吸收。我们合成的 KNTO 不仅将 TiO_2 对光的吸收从不可见光扩展到可见光，此种材料的双吸收进一步增强了对光的响应。对污染物亚甲基蓝的吸附 30min 和光催化降解 20min 后达到 79%，降解机理如下图。



图：KNTO 对 MB 的光催化降解机理

关键词：水热制备，KNTO 纳米片，层状钛酸盐，双吸收，光催化

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M-P030

专题代码：M

Tuning the electronic properties by strain and external electric field in armchair Janus MSSe (M=Mo, W) and MoSSe/WSSe superlattice nanoribbon: A First-Principles Study

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Abstract: Motivated by the successful synthesis of Janus monolayer MoSSe [1-2], we systematically study armchair MoSSe nanoribbons (A-MoSSe NRs), WSSe nanoribbons (A-WSSe NRs) and MoSSe/WSSe superlattice nanoribbons (A-SLNRs) and investigate the electronic properties modulated by the strain and external electric field using the first-principles calculations. The pristine A_3-MSSe NR (M=Mo, W) and A_3-SLNR are nonmagnetic semiconductor with indirect and direct bandgap, respectively. In the strain range of -10% to 10%, their bandgap can be gradually reduced from about 1.34 to 0.78 eV, and the bandgap is more sensitive to tensile strain than compressive strain. Moreover, the band structure of A_3-MoSSe NR and A_3-WSSe NR change from indirect character to direct at Γ point under the tensile strain of 2% and 6% due to the shift of the energy states near the Fermi level, respectively. The A_3-SLNR maintains its direct bandgap under strain. Under an external electric field, their bandgap decreases a little at first within 0.4 V/Å and then decrease a lot with the increase of

external electric field, until it becomes metallic at 0.6 V/Å. Our calculations show that the electronic properties of A_3-MSSe NR (M=Mo, W) and A_3-SLNR can be controlled by applying strain and external electric field, indicating their potential applications to nanodevices.

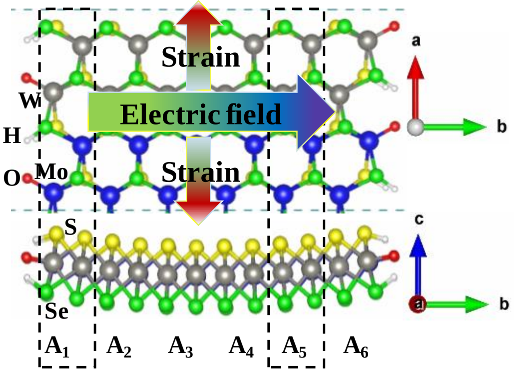

Figure 1 Side and top view of the structure of the MoSSe/WSSe superlattice nanoribbon composed by MoSSe and WSSe in a direction, defining the ribbon width along b direction (A_1, A_2 …). The Mo, W and S, Se at the edge are saturated with O and H atoms, respectively.

Key Words: Transition metal dichalcogenide, Strain, Electric field, Electronic properties, Superlattice

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M-P031

专题代号：M

四元全赫斯勒合金 HfCoCrAl 的第一性原理研究

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摘要：半金属材料因其不同于常规磁性材料的能带结构而被广泛研究。具体的说，对于上自旋电子而言，体系表现出导体的性质；而对下自旋电子而言，体系表现出半导体/绝缘体的性质，即随这电子自旋方向的不同而表现出不同的输运性质。迄今为止，虽然大量的半金属材料或从理论上被预测或在实验中得以证明，但寻找具有更高居里温度和大半金属带隙的半金属材料仍然是自旋电子学领域的热点之一。

我们采用全势-线性化缀加平面波方法对四元赫斯勒合金 HfCoCrAl 的电子结构和磁性进行了研究。通过计算确定了该材料铁磁态相较于反铁磁态和顺磁态更加稳定态。该材料的稳定态晶格常数为 6.12 Å。该合金的总磁矩为-3.23μB，其磁性主要源于 Co 原子和 Cr 原子的 3d 轨道的自旋劈裂。虽然稳定态

时该材料并不具有半金属性质，但可以通过外界压力诱导半金属性质的产生。如图 1 所示，当该材料晶格收缩时，上自旋态密度几乎不变，下自旋态密度向高能量方向移动，当晶格压缩为率 1%时，对于体系表现出半金属性质，总磁矩为-2.00μB。而当晶格膨胀时，下自旋态密度几乎不变，上自旋态密度向高能量方向移动，当晶格压缩为率 3%时，体系表现出半金属性质-4.00μB。由此可见该材料可以通过晶格大小的调节实现不同自旋电子的通过。

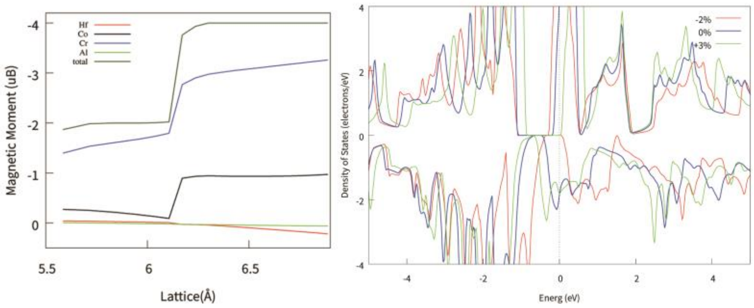

图 1 四元赫斯勒合金 HfCoCrAl 总磁矩以及原子磁矩与晶格的关系（左）总态密度与晶格参数（右）

关键词：赫斯勒合金，半金属，第一性原理

参考文献

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基金项目：中南民族大学中央高校基本科研业务费专项资金资助（CZY19009）

M-P032

专题代号：M

氢在钯金属表面吸附扩散过程的机理研究

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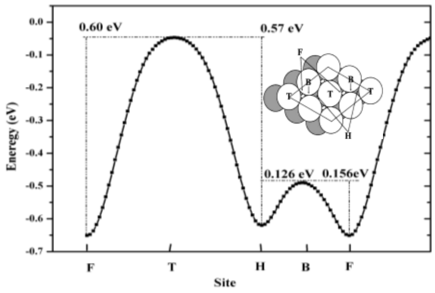
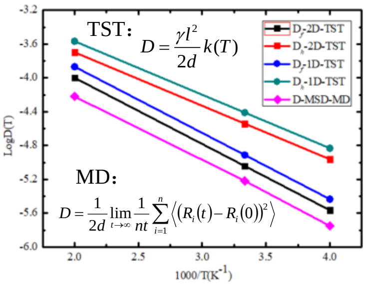
摘要：随着社会能源问题的加重，能源和化工产业正面临着向高效、低碳和环保等方向的重大变革，这要求催化反应能有更高的活性和更高的选择性。Pd 是一种优良的储氢材料，是氢能以及燃料电池技术中的一种重要催化剂材料。在实际反应中，无论是加氢反应还是氢的存储纯化，都要从氢原子/分子与 Pd 表面的接触开始，经历吸附、扩散等过程。过程中，H 在 Pd 表面的吸附状态、吸附位、吸附难易程度、在表面的迁移性、电荷迁移情况、对表面结构的影响等都将对反应速度和反应方向起到关键作用。

因此对氢与 Pd 金属表面的相互作用机理进行深入研究以达到可以理性设计催化剂活性中心从而让催化反应朝着期望的方向进行是当今催化研究的重要课题之一。

课题组团队采用第一性原理计算，通过精确构建势能面的方法，系统研究了氢分子在 Pd(111)表面上分解吸附的氢原子覆盖度效应，发现在同一覆盖度下氢原子依据吸附位置的不同会对氢分子的分解产生毒化和促进两种相反的作用，并提出了一个可以有效预测不同吸附原子构型表面活性变化的分类统计方法。同时，发展了高效且转移性较好的可用于描述氢与钯金属表面相互作用的反应力场势（二阶矩反应力场和键序势反应力场），在此基础上结合分子动力学方法计算模拟了氢在钯金属表面的吸附、扩散的动力学行为，使用动力学模拟结果验证了过渡态理论计算扩散系数的精确性，提出了可分析原子双势垒扩散问题的有效方法。





关键词：氢钯体系 吸附扩散动力学 双势垒扩散

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基金项目：江苏省高等学校自然科学研究面上项目（NO.: 18KJB140004）

M-P033

专题代号：M

Kinetic pathways towards mass production of singlecrystalline stanene on topological insulator substrates

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Abstract:As a highly appealing new member of the two-dimensional (2D) materials family, stanene was first epitaxially grown on a three-dimensional topological insulator of Bi2Te3; yet, to date, a standing challenge is to drastically improve the overall quality of such stanene overlayers for a wide range of potential applications in next-generation quantum devices. Here we use state-of-the-art first-principles approaches to explore the

atomistic growth mechanisms of stanene on different Bi2Te3(111)-based substrates, with intriguing discoveries. We first show that, when grown on experimentally studied Te-terminated Bi2Te3, stanene would follow an unusual partial-layer-by-partial-layer growth mode, characterized by short-range repulsive pairwise interactions of the Sn adatoms; the resultant stanene overlayer is destined to contain undesirable grain boundaries. More importantly, we find that stanene growth on Bi2Te3(111) pre-covered with a Bi bilayer follows a highly desirable nucleation-and-growth mechanism, strongly favoring single crystalline stanene. We further show that both systems exhibit pronounced Rashba spin–orbit couplings, while the latter system also provides new opportunities for the potential realization of topological superconductivity in 2D heterostructures. The novel kinetic pathways revealed here will be instrumental in achieving the mass production of high-quality stanene with emergent physical properties of technological significance.

M-P034

专题代号：M

New carbon allotropes identified in stochastic group and graph constrained searches by RG2 code

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摘要: RG2 is a high-efficient code, based on Random strategy combined with space Group and Graph theory, to generate crystalline structures with well-defined structural features [PRB, 97, 014104 (2018)].This poster shows two new stories about applying RG2 to search novel carbon allotropes. The first one is about a novel 3D cubic carbon allotrope (I-43d) in sp3 hybridization with large-size (188 atom per cubic cell) and low-energy [112 meV/atom higher than that of cubic diamond]. It is a super-hard insulator with an indirect band gap of 7.25 eV, which is the largest band gap in present carbon family [PRL, 121, 175701 (2018)]. The second one is about the discovery of 33 new 2D carbon allotropes including a novel Stone-Wales graphene with intriguing structure (well-arranged Stone-Wales defects) and remarkable stability exceeding than all the previously proposed 2D carbons. It can be constructed through a 90o bond rotation in a 8×8 supercell of graphene, which is a “magic size” showing better stability than those based on 9×9, 12×12 and 13×13 supercells. Such a “magic size” can be simply understood through a “energy splitting and inversion” model. The calculated vibrational

properties and molecular dynamics of SW-graphene confirm that it is dynamically stable. The electronic structure shows SW-graphene is a semimetal with distorted, strongly anisotropic Dirac cones [PRB, 99, 041405 (R), 2019].

关键词：Crystal structure searching; Carbon allotropes; RG2.

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M-P035

专题代号：M

二维碲材料的结构，拓扑，和超导性质的第一性原理计算研究

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摘要：继石墨烯，磷烯，和硼烯的发现和制备之后，碲烯在理论上的预测[1]和实验上的成功制备使单质二维材料的范围扩展到了第六主族元素，而碲烯在新一代的电子和光电器件中也具有十分巨大的潜在应用价值。我们通过粒子群优化算法结合第一性原理密度泛函理论计算，进一步地预言了 31 种具有不同结构特征的二维碲的同素异形体。根据这些新的二维碲结构的原子层数，它们被分为了四类并被命名为 M-α，B-α，T-α，T+α 等。我们通过声子谱计算验证了这些新的碲烯结构的动力学稳定性。我们的计算也表明这些新的结构具有各种各样的电子性质，包括金属性质，半导体性质，拓扑性质和超导性质。其中，B-α，B-β，B-γ，和 B-η 具有拓扑绝缘体性质，B-β, B-ε 和 T-κ 具有本征超导性质（超导转变温度约为 8 K）。值得一提的是，B-β 同时具有拓扑性质和超导性质，这可能是第一个同时具有拓扑性质和本征超导性质的材料，为研究二维系统中的拓扑超导体提供了平台。我们的研究结果为将来理论上预言和实验上合成新颖的二维碲结构打下了坚实的基础。

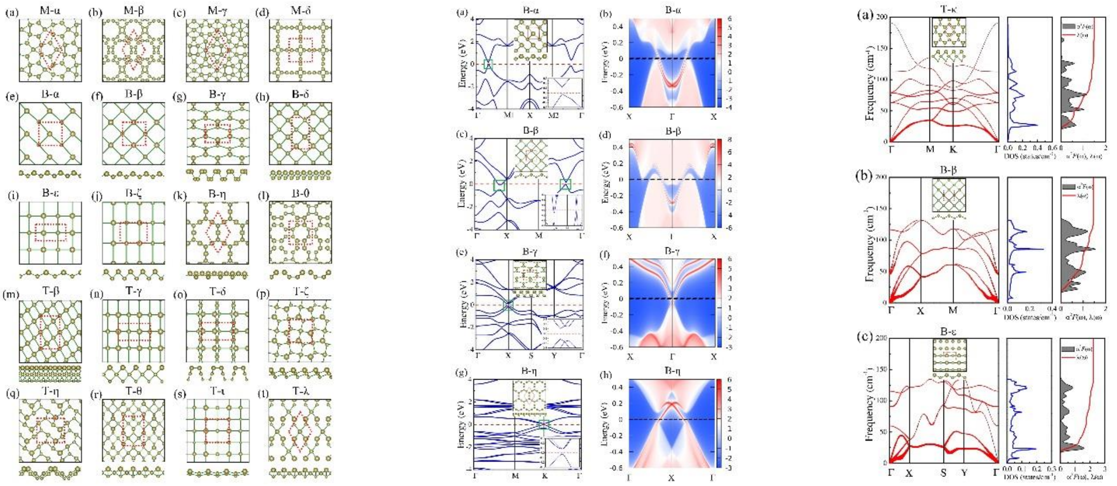

图 1. 由左至右分别为：预测的部分碲烯的结构图；B-α ,B-β 和 B−ζ 的能带结构和边缘态结构；T-κ, B-β，和 B-ε 的声子谱，声子态密度，Eliashberg 函数，和电声耦合常数。

关键词：二维材料，碲烯，拓扑，超导

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基金项目：国家自然科学基金（NO. 11504332, NO. 11774078)

M-P036

专题代号：M

第一性原理研究 T1 相的腐蚀机理

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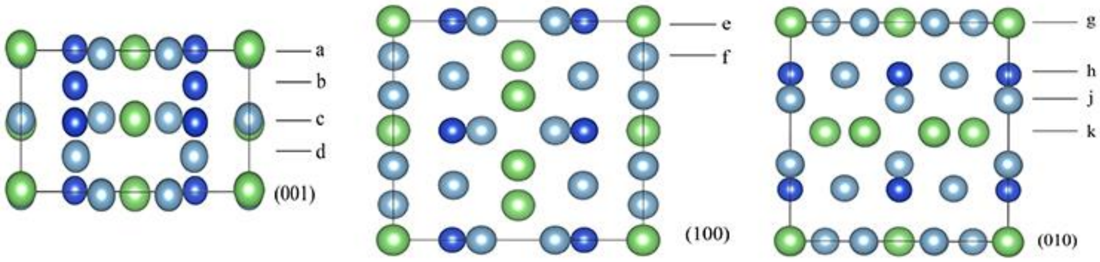
摘要：在 Al-Cu-Li 三元体系里，铝中 Li 的加入降低了合金的密度，增加了合金的刚度，而与 Cu 的结合促进了析出强化，从而获得了高强度的沉淀析出物[7, 8]。在众多的析出物中，T1 相是主要的强化析出物,它是常见并且深入研究的中间相之一。实验研究表明，T1 相对 Al-Cu-Li 合金的腐蚀起着关键作用，研究 T1 相的腐蚀机理具有重要的意义。研究 Al-Cu-Li 合金体系腐蚀机理，其前提是获得合理可信的 T1 相晶体结构。事实上，已有大量的实验和理论工作构建和预测 T1 相的晶体结构，提出了一种新的 T1 相合理结构($Al_6Cu_4Li_3$)，使得原子长度尺度上的 T1 相的研究成为可能。

为了进一步揭示 T1 相的腐蚀机理，本文从电子层面入手，利用密度泛函理论结合表面能、电子功

函数研究不同终结面的表面稳定性，针对 T1 相的不同面，讨论了应力对其影响，同时计算了 Ag，Mg 和 Zn 在 Al/T1 界面替位能以此讨论合金元素对 T1 相析出的影响。研究发现，表面电子功函数与终结面原子种类有关，Li 由于其电负性最小，含 Li 终结面的功函数会更低，进而降低了材料的耐蚀性。应力条件下 T1 相的腐蚀与纯金属的腐蚀存在差别，这主要是因为 T1 属于三元合金相，并不是纯金属块体相。并且 T1 相界面处存在一定的晶格畸变，有益于参杂原子偏聚，且 Ag 与 Al 半径最相近，替位能最低，因此 Ag 更容易促进 T1 相形成，以降低材料的耐蚀性。



关键词：Al-Cu-Li 合金；T1 相；电子功函数

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基金项目：国家自然科学基金项目（No. 2014GXNSFFA118004）

M-P037

专题代号：M

Low Frequency Acoustic Phonon Ehenced Negative Thermal Expansion in $M^{II}_2[M^{IV}(CN)_8](M^{II}$=Ni, Co, Fe, Mn; M^{IV} =Mo, W) from *Ab Initio* Calculations

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Abstracts：Ni2W(CN)8 is the first reported experimentally solid material showing negative thermal expansion(NTE) recently. Here, by using first-principles calculations within density functional theory (DFT) combined with the quasi-harmonic approximation (QHA) theory, we investigated systematically the NTE properties for MII2[MIV(CN)8](MII=Ni, Co, Fe, Mn; MIV =Mo, W) family. We show that the coefficients of negative thermal expansion (CNTE) of MII2[MIV(CN)8] can reach up to ~ -10 × 10-6 K-1, i.e., Ni2W(CN)8, Ni2Mo(CN)8 and Mn2W(CN)8 are -9.14 10-6 K-1, -8.61 × 10-6 K-1 and -14.77 × 10-6 K-1 respectively. Analysis of the derived Grüneisen parameters reveal that, like most Prussian blue analogues, the optical modes make a contribution to the NTE, which involve the localized rotational motion of the WC8 units and the transverse vibration of CN in an approximately two-dimensional plane. Moreover, we also find that the low frequency acoustic modes from Γ(0 0 0) to X(0.5 0 0) make a significant contribution to the NTE of MII2[MIV(CN)8] family. The eigenvectors for these modes reveal an almost rigid transverse motion of both NiN4 and WC8 unit, and the whole transverse vibration induces a slight ripple to reduce the volume, similarly as membrane effect in graphene. Our results present a clarity picture for the driving mechanism of NTE in Ni2[MIV(CN)8], and provide a guide to adjust the CTEs by element substitution in experiment further.

Key words: negative thermal expansion   octacyanido-based cyanide   Ab Initio Calculations

M-P038

专题代号：M

Thermal Tuning of Acoustic Manipulation by a Ferroelectric Phononic Crystal Plate

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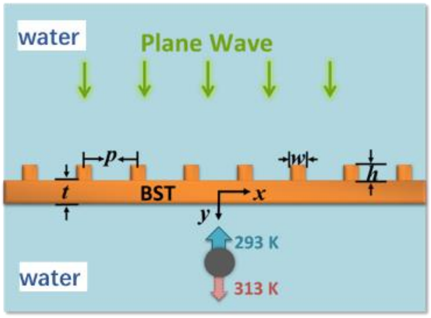
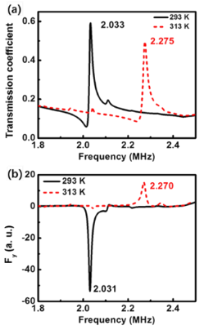
Abstrct: We investigated a tunable PCP made of $Ba_{0.7}Sr_{0.3}TiO_3$ (BST) ceramics, wherein a 20-K temperature change near room temperature results in a 20% frequency shift in the transmission spectra induced by a ferroelectric phase transition.[1] Though PCP made of $Ba_{0.7}Sr_{0.3}TiO_3$ (BST) were studied as thermal tunable PCP by some researchers, most of the researches focus on the intrinsic properties. It is meaningful to discover more manipulation capability of the tunable PCP which is potential in many applications such as biomedicine, chemosynthesis and sensor. In this article, we report a thermal tuning of acoustic manipulation by a subwavelength-scale (relative to the wavelength of ultrasound in water) ferroelectric PCP. The longitudinal velocity and transverse velocity of BST increase nonlinearly and progressively from 293 K to 313 K, because the tetragonal-cubic phase transition occurs across the Curie temperature (298 K). We studied numerically the ARF on a cylindrical brass particle near the surface of a periodically structured BST plate and investigated the capability of acoustic trapping versus two different temperatures (293 K and 313 K). It is demonstrated that this system traps (negative acoustic radiation force) a particle well around the surface at 293 K, whereas pushes (positive acoustic radiation force) the particle away from the surface at 313 K. The mechanism is revealed that the gradient vortex velocity field at 293 K turns to be a uniform periodic velocity field at 313 K by analyzing the band structures and field distributions. The thermal tuning acoustic manipulation is a novel tool of micro-scale particle manipulation, which contributes to more smart devices and inspires more researches of unused tunable acoustic manipulation.





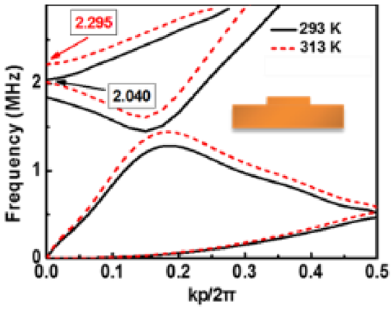


FIG. 1. Schematic representation for thermal tuning of acoustic radiation force by a $Ba_{0.7}Sr_{0.3}TiO_3$ phononic crystal plate.

FIG. 2 (a) Transmission coefficient versus frequency in 293 K (black solid line) and 313 K (red dash line). (b) Acoustic radiation force on particle versus frequency in 293 K (black solid line) and 313 K (red dash line).

FIG. 3. Band structure of $Ba_{0.7}Sr_{0.3}TiO_3$ phononic crystal plate in 293 K (black solid line) and 313 K (red dash line). The inset is schematic diagram of the single unit for intrinsic band structure calculation by finite element method.

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基金项目：国家自然科学基金项目（NO. 11874286，11774057）

M-P039

专题代号：M

Superconducting Single-Layer T-Graphene and Novel Synthesis Routes

单层 T-Graphene 的超导及其合成路径

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摘要：单层超导体是制备超导纳米元器件的理想材料，然而目前已知的单层超导体很少，只有单层的二硒化铌、二硫化钼和铁硒等。另外，单层的元素超导体就更为少见，理论预言的超导二维硼到目前还没有在实验上测到超导。所以，寻找和合成单层超导体，特别是单层的元素超导体，一直是大家非常感兴趣的课题。最近，“魔角石墨烯”中超导的发现使这个课题受到更多的关注。碳元素具有丰富的电子杂化构型，使它呈现很多的同素异构体。每一种碳元素同素异形体的出现都会引起极大的研究热潮，如富勒烯、碳纳米管、石墨烯等。另外，碳材料的超导也一直是大家非常关心的课题，包括石墨插层化合物中的超导，但它们的超导转变温度一般都不高。我们课题组利用晶体结构搜索和第一性原理计算在碳的同素异构体中找到一种本征的单层超导体 T-graphene。这种单层碳材料具有四八环结构，他们的电声子耦合计算表明，单层 T-graphene 在常压下的超导转变温度可以达到约 20.8 K。更为重要的是，他们首次提出了“高压合成，常压剥离”的思路，设计了两条巧妙的路径来获取这种新奇的材料（图 1）。第一条路

径是，先用高压方法（> 11.5 GPa）合成碱金属钾和碳的化合物，具有 P4/mmm 对称性的 C4K。计算表明这种化合物在高压下稳定，并在压力撤掉后仍是一个亚稳相。接下来用电化学方法或机械剥离法从 C4K 中把单层 T-graphene 剥离出来。第二条路径是，在常压下将钾原子从 C4K 中蒸发掉，留下纯的 T-graphite 层状物（C4），接着从 T-graphite 中剥离出 T-graphene，此时的剥离能比直接从 C4K 中剥离更低。他们用多种方法证明了 C4K 在高压和常压下的稳定性，以及单层 T-graphene 剥离的可行性。他们还预言，C4K 本身也是一种超导体，其理论计算的超导转变温度达到近 30 K，是目前类似石墨插层化合物中超导转变温度最高的材料。他们的研究表明，C4K 和 T-graphene 都具有很强的电声子相互作用，属于常规超导体，可以用电声耦合的方法来研究它们的超导电性。

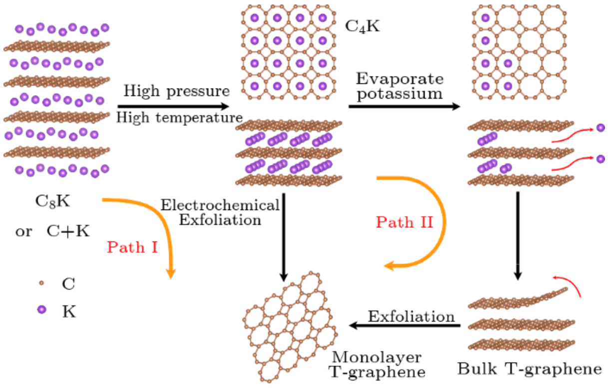

图 1. 单层碳元素超导体 T-graphene 的合成路径示意图，简单阐明了“高压合成，常压剥离”的新思路

关键词：单层超导体 高压 单层 T-graphene 第一性原理

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M-P040

专题代号：M

Pressure-Stabilized High-Energy-Density Alkaline-Earth-Metal Pentazolate Salts

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Abstract：Polynitrogen compounds especially pentazolate anion complexes recently have attracted substantial attention due to their promising potential as high-energy-density materials. Here, using a machine-learning-accelerated crystal structure search method and first-principles calculations, we predict a new hybrid compound by inserting a large fraction of nitrogen into alkaline-earth metals. It is a new stoichiometric type MN_{10} (M = Be, Mg), which possesses a metal-centering octahedral pentazolate framework with the space group *Fdd*2. This type of ionic-like molecular crystal is found to be energetically more favorable than the mixtures of M_3N_2 or MN_4 compounds and pure nitrogen and is possibly synthesized at relatively low pressures (around 12 GPa for MgN_{10}). The ab initio molecular dynamics simulations show that they are metastable and can be quenched to ambient conditions once synthesized at high pressure. Moreover, decomposition of this polymeric MN_{10} structure can release a large amount of energy and shows high performance in detonation. The detonation velocity and pressure of BeN_{10} are about twice and 4 times that of trinitrotoluene, respectively.

Key words: Crystal structure searching, High pressure, High energy density, Pentazolate

Reference: 【1】 K. Xia *et al.*, Pressure-Stabilized High-Energy-Density Alkaline-Earth-Metal Pentazolate Salts, *J. Phys. Chem. C* 2019,123 (16), 10205.

Funds: MOST of China (Grant Nos. 2016YFA0300404 and 2015CB921202), National Natural Science Foundation of China (Grant Nos. 11574133 and 11834006), Science Challenge Project (No. TZ2016001), the NSF of Jiangsu Province (Grant No. BK20150012), the Fundamental Research Funds for the Central Universities, and Special Program for Applied Research on Super Computation of the NSFC-Guangdong Joint Fund (the second phase).

M-P041

专题代号：M

Multiple superionic states in helium-water compounds

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ABSTRACT: Superionic states are phases of matter that can simultaneously exhibit some of the properties of a liquid and of a solid. For example, in superionic ice, hydrogen atoms can move freely while oxygen atoms are fixed in their sublattice. “Superionicity” has attracted much attention both in fundamental science and applications. Helium is the most inert element in nature and it is generally considered to be unreactive. Here we use ab initio calculations to show that He and H2O can form stable compounds within a large pressure range which can exist even close to ambient pressure. Surprisingly, we found that they can form two previously

unknown types of superionic states. In the first of these phases the helium atoms exhibit liquid behavior within a fixed ice-lattice framework. In the second of these phases, both helium and hydrogen atoms move in a liquid-like fashion within a fixed oxygen sublattice. Because the He-O interaction is weaker than the H-O interaction, the helium atoms in these superionic states have larger discussion coefficients and lower “melting” temperatures than that of hydrogen, although helium is heavier than hydrogen. The insertion of helium atoms substantially decreases the pressure at which superionic states may be formed, compared to those in pure ice.

M-P042

专题代号：M

Ground States of Au_2Pb and Pressure Enhanced Superconductivity

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ABSTRACT: Au_2Pb was suggested to be a natural topological superconductor and has attracted much attention. Combining ab initio calculations with machine-learning accelerated crystal structure searches, we find two new ground states: Pca21 phase at ambient pressure and I-42d phase at high pressure. The Pca21 phase is energetically more favorable than the Pbcn structure previously suggested, and in better agreement with the experimental XRD pattern. Our calculations suggest that the high-pressure I-42d is a phonon-mediated BCS superconductor. By the high pressure electric resistance measurements, we observe a strong enhancement of Tc at a factor of more than three times than in the low-pressure case. Tc reaches a maximum value of around 4 K at 5 GPa and then decreases with further compression. The superconductivity can remain unchanged after the pressure is released, in consistence with our theoretical predictions. These results show that Au2Pb exhibits abundant behaviors under pressure and temperature, which can help to understand how to adjust its electronic properties by pressure.

M-P043

专题代号：M

Improve the performance of Machine-Learning Potentials by optimizing descriptors

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ABSTRACT: We have implemented Behler-Parrinellodescriptors in a differentiable way and fitted force fields of Aluminum by Gaussian approximation potential (GAP) . Our method can effectively improve the performance of ML interatomic potentials in different systems such as bulk and grain boundaries.

M-P044

专题代号：M

二氧化钛界面光生载流子激发态动力学

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ABSTRACT： TiO_2 is an intensively studied photocatalytic material owing to its low cost and high activity. The anatase/rutile (A/R) mixed-phase TiO_2 is recognized as an effective strategy to achieve high photocatalytic efficiency by the type-II band alignment favorable to spatial charge separation. However, the atomic structure, as well as the exact band alignment of the A/R mixed-phase TiO_2, is very difficult to identify either in experimental measurements or theoretical simulations. Moreover, the time-dependent photogenerated carrier dynamics, which can determine the photocatalytic efficiency, has not been studied at the atomic scale. In this report, we use adaptive genetic algorithm to search the stable interface structures. We find that the band alignment is determined by the interfacial atomic structures. Especially, with oxygen vacancy (O_V) at the interface, band alignment can be reversed as compared to that of the stoichiometric interface. Then, we select one stoichiometric and one defective structure to study the photogenerated carrier dynamics using the time-dependent *ab initio* nonadiabatic molecule dynamics. We find that in the stoichiometric system, for both the electron and the hole, the charge transfer happens within 400 fs, which is much shorter than the electron-hole recombination timescale at ns to μs magnitude, which suggests that the charge transfer can occur efficiently at the interface before they recombine. For the defective A/R system with O_V, we find that the electron will be trapped by the defect state within 1 ps, while the hole dynamics is not affected. Our study provides atomic insights into the understanding of the band alignment and photogenerated carrier dynamics at the mixed A/R TiO_2 interface, which provides valuable guidance for functional material design for solar energy conversion.

KEYWORDS: band alignment , photogenerated carrier dynamics, electron-hole recombination

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M-P045

专题代号：M

High-pressure study of the structural phase transition in $Cu_{1.875}Te$

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$Cu_{2-x}Te$ is one of the commonly used as conductive back contacting materials for CdTe solar cells due to the formation of p+ interface with CdTe absorber. Because of the unavoidable Cu deficiencies, complex structures relating closely with Cu contents have been reported for $Cu_{2-x}Te$ till now, which limited the study on its broad application. Here, combining X-ray diffraction (XRD) measurement with extensive swarm structure search, we proved P-3m1 phase as the ambient structure of $Cu_{1.875}Te$ and it will transform to a new defective $I4/mmm$ phase at 2.9 GPa. Enthalpy calculation supports that stoichiometric Cu_2Te is expected to be synthesized under high pressure above 5.3 GPa. The analysis of mechanical and dynamical stability implies that the high-pressure $I4/mmm$ Cu_2Te has potential to be stabilized to ambient conditions as a metastable material. Our results represent a significant step in understanding the crystal information of $Cu_{2-x}Te$ and extending its applications.

Keywords: phase transition; crystal structure prediction; high-pressure experiment; copper deficiencies

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M-P046

专题代号：M

Hydrogen as a source of flux noise in SQUIDs

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Superconducting circuits have a wide variety of applications, e.g., photon detectors used in astrophysics, bolometers involved in dark matter searches, nanomechanical motion sensors, cavity quantum electrodynamics, and quantum limited parametric amplifiers. However, their performance continues to be impaired by noise and dielectric loss produced by microscopic defects. Of particular interest as a qubit is the superconducting quantum interference device (SQUID) where a major problem is low-frequency 1/*f* flux noise generated by fluctuating spins residing on the surface. These surface spins comes from a variety of microscopic sources. Recent experiments indicated that hydrogen (H) atoms may be one of those sources, even though hydrogen is rarely associated with magnetism.

In this work, we used density functional theory (DFT) to investigate H atoms as a source of flux noise on α-Al_2O_3(0001), which is the insulating parts of Al based SQUID. We found that H atoms either embedded in, or adsorbed on, an $\alpha-Al_2O_3$(0001) surface have sizable spin moments ranging from 0.81 to 0.87μB with energy barriers for spin reorientation as low as ∼10mK. Furthermore, H adatoms on the surface attract gas molecules such as O_2, producing new spin sources. We propose coating the surface with graphene to eliminate H-induced surface spins and to protect the surface from other adsorbates.

Key words: Superconducting qubit, 1/*f* flux noise, Density functional theory

Reference:

【1】 Z. Wang *et al.*, Hydrogen as a source of flux noise in SQUIDs, *Phys. Rev. B* 2018, 98, 020403(R).

Foundation: National Science Foundation of China under Grant No. 11474056 and National Basic Research Program of China under grant number 2015CB921400.

M-P047

专题代号：M

Ellipticity Dependence of Third-Order Nonlinear Optical Response of GrapheneIrradiated by Two-Color Lights

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ABSTRACT: Graphene is a massless Dirac fermions system where electrons move at 106m/s. At the hexagonal Brillouin zone corners, that is, near the Dirac point, the band structure of graphene represents linear dispersion relationship. For this reason, the nonlinear properties of graphene plays an essential role due to its linear dispersion. It has been discussed and investigated theoretically and experimentally that graphene has stronger nonlinearity than what in dielectric medium or traditional semiconductor. In recently years, nonlinear response enhancement of graphene under elliptical electric field has been observed and investigated. Third or fifth order response of graphene monotonically decrease with increasing of ellipticity from 0 to 1 while seventh order response reaches a peak at special ellipticity of 0.32. In this work, we consider graphene is radiated by a two color lights with two different frequency ω0 and 2ω0, sum frequency and slip frequency of third order response will generate 3ω0 harmonic with two different contribution.This difference from one light radiation leads tounique phenomenon in dependence of intensityI(3ω0) on ellipticity.

M-P048

专题代号：M

Coexistence of Superconductivity with Enhanced Charge Density Wave Order in the Two-Dimensional Limit of $TaSe_2$

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Abstract: Bulk 2H-$TaSe_2$ is a model charge density wave (CDW) metal with superconductivity emerging at extremely low temperature (T_c = 0.1 K). Here, by first-principles calculations including the explicit calculation of the screened Coulomb interaction, we demonstrate enhanced superconductivity in the CDW state of monolayer 1H-$TaSe_2$ observed in recent experiments. Its ground-state 3 × 3 CDW phase features triangular clustering of Ta atoms and possesses a large electron−phonon coupling of $\lambda = 0.74$, yielding an order of magnitude higher superconducting T_c compared to the bulk. Upon lowering the thickness from bulk to monolayer $TaSe_2$, the CDW intensifies with slightly decreased Fermi-level density of states, while superconductivity gets boosted via a largely increased intrinsic electron−phonon coupling strength, which overcomes both the CDW effect and naturally reinforced Coulomb repulsion. These results uncover the simultaneously enhanced CDW and superconducting orders in the two-dimensional limit for the first time and have key implications for other CDW metals like 2H-TaS_2.

关键词：$TaSe_2$, charge-density wave, superconductivity, transition-metal dichalcogenide

基金项目：国家自然科学基金项目（51788104, 11674188, 11874079, and 11847116）等

M-P049

专题代号：M

A type-II C_2N/α-Te van der Waals heterojunction with improved optical properties by external perturbation

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Abstract: C_2N with uniform honeycomb holes and nitrogen lattice, whose vacant sites are partially filled by C_6 hexagons, have great potential for editable properties. Here, by using the first-principles calculations, C_2N/α-Te van der Waals (vdW) heterojunction and its electronic properties modulated by vertical strain and external electric field have been systematically investigated. The results show that the C_2N/α-Te vdW heterojunction has a unique type-II band alignment, whose indirect band gap value is 0.47/1.01 eV in DFT/HSE06. The band gap can be tuned by external electric field and vertical strain from 0.49 eV to 1.16 eV in HSE06. A type-II to type-I transition occurs under external electric field of in 0.4 V/Å. Interestingly, C_2N/α-Te vdW heterojunction possesses high optical absorption strength and broad spectrum width (ultraviolet to near-infrared). These results indicate that the C_2N/α-Te heterojunction will have promising applications in photoelectron and photovoltaic applications.

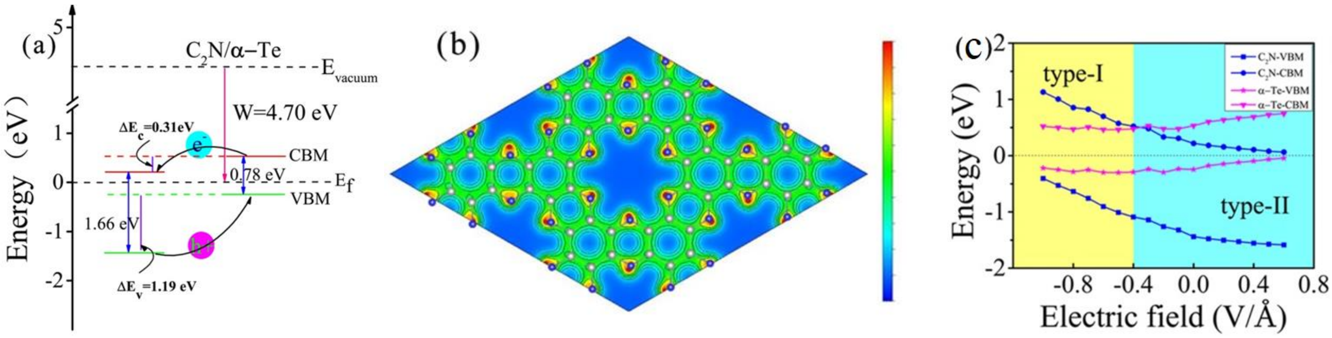

Fig. 1 (a) The band alignment of the C_2N/α-Te heterojunction. (b) 2D charge density distribution of C_2N/α-Te heterojunction at C_2N surface. (c) The band edge as a function of the external electric field in the C_2N/α-Te heterojunctions.

M-P050

专题代号：M

Monolayer MoS_2 Adsorbed on Transition Metal substrate for Highly Efficient Single-Atom Catalysis of CO Oxidation design

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ABSTRACT: Developing highly efficient single-atom catalyst (SAC) is of great scientific and technical importance due to the high efficiency and specificity for many chemical reactions. Using first-principle calculation within density theory, we investigate a powerful strategy for decreasing the instability of SACs by tuning the electronic interactions of metal and sub substrate. It is identified that, the Pd2 dimer is prone to dissociate with a single-layer MoS2 adsorbed on Au(111), Ag(111) two representation transition metal substrate having 5.18% (mismatch) tensile strain with the MoS2 overlayer. The straining provide by metal substrate induces a semiconductive-to-metallic phase transition of the MoS2 overlayer substrate. Moreover, elements as Pd Cu, and Mn , can also be stabilized into high performance SACs for CO oxidation with tunable reaction barriers. The present findings may prove to be instrumental in development of highly cost-efficient and high loading density of SACs stability on MoS2 overlayer substrate.

Key words: Single atom catalyst, Charge transfer, defect-free 2H-MoS2, strain engineering, electronic metal-substrate interactions, CO oxidation, dnesity functional theory.

M-P051

专题代号：M

Large Magnetic Anisotropy Energy and Valley Splitting Energy of Single Transition Metal Ad-atoms on Monolayer WS_2

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Abstract

Atomically thin 2D material absorbed with a single magnetic atom hold out the promise to overcome the difficulties of bit miniaturization for data storage. One key issue is to find out an appropriate material system with high structural stability and large magnetic anisotropic energy. In this letter, we perform density functional calculations and demonstrate perpendicular magnetic anisotropy energy up 30 meV/atom (above room temperature) in rhenium atom adsorbed on monolayer tungsten disulfide, which makes this system a promising candidate for achieving the single ad-atomic systems for applications of magnetic data storage.

Furthermore, the local magnetic moments are introduced into the system via rhenium adsorption, which leads to Zeeman Effect, and can further lift the valley degeneracy. The large valley splitting energy generated by transition metal atom adsorption offers a novel paradigm for the development of valleytronic devices.

Keywords: information storage; transition metal ad-atom; magnetic anisotropy energy; valley splitting

基金项目： 国家自然科学基金项目（NO. 11474056）

M-P052

专题代号：M

Spin-polarized current in wide bandgap hexagonal boron nitrides containing 4|8 line defects

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Abstract: Since the discovery of graphene, the study of atomically thin two-dimensional (2D) nano materials has become one of the most rapidly developing areas of condensed matter physics for pursuing the novel properties, rich low-dimensional physics and the abundant applications. 2D materials are considered as the promising candidates for the innovation of integrated circuits due to the availability of their versatile electrical properties, spanning from insulator, semiconductor to metal and superconductor, a broad range of material parameter space. Hexagonal boron nitride (*h*-BN) monolayer has honeycomb lattice structure, sharing the similar planar hexagonal structure to graphene. Whereas the former possesses a wide bandgap of about 4.5 eV.

Line defects which commonly present in two-dimensional materials can play a fundamentally important role in spintronic applications for generating and transporting spin current. Electrical controllability and room-temperature magnetism are two important ingredients for spintronics device applications. By combining density functional theory with the nonequilibrium Green's function method, we investigate theoretically the electronic and magnetic properties of n-type doped monolayers of boron nitride (h-BN) with 4|8 line defects. We show that the line defects create two deep flat bands in the large band gap of the h-BN sheet, inducing van Hove singularities in the density of states. It is well known that a sharp van Hove singularity (VHS) on the DOS can appear at the band edge in a 1D dispersive band. Interestingly, at certain concentration of electrons introduced by n-type doping a tantalizing spontaneous one-dimensional ferromagnetic ordering along with such line defects in the h-BN sheet emerges. The net magnetic moment of the system emerge sharply at the critical doping level around 7.08×10^{13} cm^{-2} (near 0.5 electrons per unit cell), and remarkably, it saturates (1 μ_B per electron) very quickly. This magnetic ordering originated from the partially occupied dispersionless conduction band (upper defect band) results in spin-polarized current. Moreover, the electron doping can be realized by replacing the B atoms with the C atoms. And the value of spin polarization efficiency (SFE) is about 90% within the bias range of 0.0-0.4 V at room temperature. This exhibits high spin polarization and the attractive spin-polarized transport behavior appears. Our findings not only reveal the possibility of doping-induced tunable magnetism in 2D semiconductors but also provide an opportunity to realize spintronics at the atomically thin single-layer level, in which controlled spin moment and transport may be achieved by electrostatic gating, which is possible to be realized experimentally.

Keywords: 2D materials, line defects, ferromagnetism, spin-polarized transport

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M-P053

专题代号：M

Data-driven descriptor for high-throughput screening of topological insulators

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Due to their salient properties, topological insulators (TIs) have immense application potential in spintronics, catalysis, and quantum computing. Such high technological expectation propels the field to actively search for new TIs. Earlier search efforts for potential TIs have been performed on a case-by-case basis. More recently, significant advances have been made in predicting new topological materials using empirical descriptors or symmetry-based indicators[1-6] that allow scanning the materials space in a high-throughput fashion. These approaches are, however, only applicable to systems with well-defined symmetries, e.g., those stored in materials databases. Hence, such approaches leave a much larger space of materials unexplored, for instance those compounds obtainable via compositional alloying. In the present work, we overcome this hurdle and show how to use artificial intelligence (AI) to uncover a novel two-dimensional descriptor for the fast and reliable identification of the topological characters of complex systems without *apriori* knowledge about their symmetries. Here, we use tetradymites as a prototypical example class of materials. The descriptor is obtained via a recently developed data-analytics approach named SISSO (Sure Independence Screening and Sparsifying Operator)[7,8] that is applied to a training set obtained via high-level electronic structure calculations. The identified descriptor is defined by only two elemental properties of the constituent species (the atomic number and the electronegativity), hence allowing us to readily scan over four million alloyed compounds in the tetradymite family. By these means, nearly two million hitherto unknown TIs are identified, thus drastically expanding the territory of the topological materials world. Moreover, these predictions are additionally verified by first-principles calculations for several representative alloyed materials, as well as by the experimental data available to date. The strong predictive power of the descriptor beyond the initial scope of the training data also attests the increasing importance of such AI-based approaches in modern materials discovery.

Keywords: topological insulators, data-driven, high-throughput screening, descriptor

M-P054

专题代号：M

Pressure-induced decomposition of binary lanthanum intermetallic compounds

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Recently, lanthanum intermetallic compounds have attracted many attentions due to their automobile and aerospace applications. It is necessary to investigate their properties under extreme conditions, such as high pressures, to further explore their potential applications. Here, we extensively examine the high-pressure properties of a series of lanthanum intermetallic compounds (M_xLa_y, M = Be, Mg, Al, Ga, In, Tl, Pb, and Bi) by using the in-house developed swarm-intelligence based CALYPSO method, which can be used to predict structures depending on the given chemical composition by merging ab-initio total-energy calculations. Although plenty of unreported high-pressure phase transitions have been identified, we find a counterintuitive phenomenon that all of these compounds will decompose into individual elements at certain pressures, which will certainly affect their applications at high pressure. In order to understand the underlying mechanisms of the decomposition, we further analyze the evolution of the internal energy and the pressure-volume term (PV term) as a function of pressure. Our results shed lights on the high-pressure behaviors of La-based intermetallic compounds and provide important guidance for other La-like intermetallic compounds.

Keywords: pressure-induced decomposition; lanthanum intermetallic compounds; crystal structure prediction

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基金项目: 国家自然科学基金项目（No.11534003, No. 11874175）

M-P055

专题代号：M

中子辐照下材料损伤的跨尺度动力学模拟

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摘要：探究中子辐照对金属材料结构和性能的影响是 CFETER 工程设计的重要根据。然而，一方面由于缺乏聚变中子源开展反应堆服役条件下的材料实验；另一方面由于实验仍然无法直接观测跨时间尺度的缺陷动力学演化过程，因此，有必要发展一套聚变堆金属材料多尺度模拟框架来预测实际服役环境下的材料行为。

课题组团队通过顺序耦合初级辐照损伤（IM3D）、原子尺度方法（DFT 和 MD）与介观尺度方法（OKMC（MMonCa）和 CD（IRadMat）），基于特征退火时间发展了一套计及空间关联效应的 CD-SC（Cluster Dynamics-Space Correlations）模型。具体地，首先将由中子能谱得到的初级离位原子（PKA）的能量和空间分布嵌入到 IM3D 程序中计算得到级联缺陷的三维空间分布；以此作为输入条件，利用开源程序 MMonCa 进行特征时间退火，为 CD 模拟提供更加准确的初始缺陷尺寸分布；最后，在 IRadMat 自主程序的基础上结合最新参数模拟缺陷的长时间动力学演化。其结果可以直接为中子辐照环境下金属材料中损伤提供理论指导和预测。

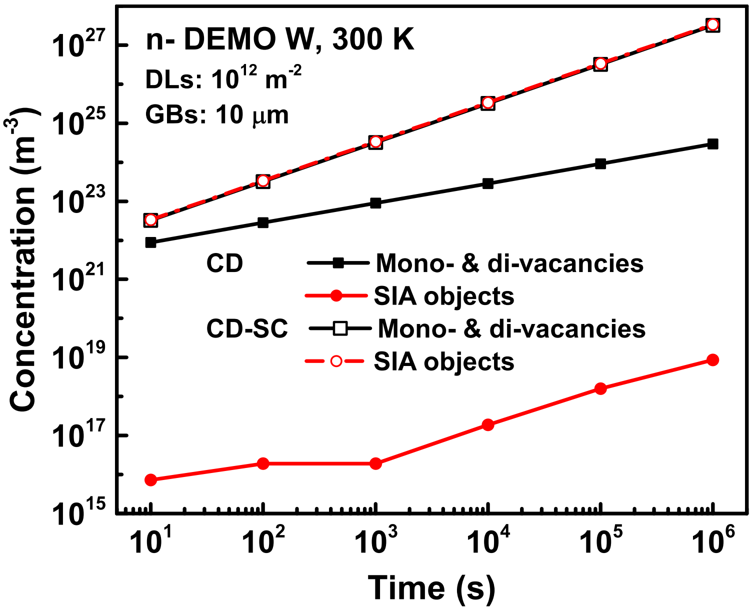

图 1 中子辐照下（DEMO）W 中缺陷密度随时间变化

关键词：中子辐照 缺陷空间关联 团簇动力学 多尺度模拟

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M-P056

专题代号：M

Robust double Weyl semimetal phase in nonmagnetic hexagonal lattice system

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摘要：We propose a simple strategy to find possible linear double Weyl semimetals (WSMs) among nonmagnetic materials. This strategy can reproduce several known robust WSM candidates, covering orthorhombic, tetragonal, and cubic lattice systems. This kind of WSM hosts Weyl points (WPs) carrying double chiral charges when spin degeneracy is considered while spin-orbit coupling (SOC) is switched off, and dispersions along all three directions are linear, distinct from the parabolic double WPs proposed in $HgCr_2Se_4$. When SOC is included, these double-charge WPs split into two single spin-1/2 WPs with equal chirality. Following this strategy and combining with ab initio structural prediction techniques, we propose a candidate for such kind of WSMs, rooted in a high-pressure phase of TiS_2 with space group *P*-62*m*. In this system, all the WPs are pinned at the same energy due to crystal symmetry. In addition, the minimum spacing between opposite-chirality WPs is ~0.23$Å^{-1}$, which makes it a promising robust WSM candidate.

关键词：Topological Weyl semimetal, high pressure, Titanium disulfide.

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基金项目：The MOST of China (Grants NO. 2016YFA0300404 and No.2015CB921202), National Natural Science Foundation of China (Grants No. 11574133 and No. 11834006), the NSF Jiangsu province in China (Grant No. BK20150012), the Science Challenge Project (Grant No. TZ2016001), and the

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M-P057

吡咯并吡咯二酮/低聚噻吩共聚物光电性质第一性原理研究

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ABSTRACT：The impact of the number of thiophenes (Th) unit on the photoelectric properties of the polydiketopyrrolopyrrole-oligo-thiophene (PDPP-NT, N = 1 - 8) was investigated with the Density functional theory (DFT). The results present that the variation of Th unit has a significant effect on electronic structure and absorption spectra. Firstly, the band gap of the PDPP-NT increases with N increase, the long wave and short wave absorption peak shows blue-shifted and red-shifted respectively, the half-height width of the absorption peak become narrow; Then, when N = 2, 3, the energy band curvature is higher than others, the corresponding effective mass is lower so that the mobility of carriers is larger; Once more, when N = 2, 3, 4 and 6, the dihedral angle are smaller than others. This indicates that the planarities of the molecular structure of the PDPP-NT (N = 2, 3, 4, 6) are better; Finally, the charge transfer between D and A units of the copolymer was analyzed with the Bader charge analysis tool. The results indicate that the gains and losses of electrons occur at the C-C vicinity between Th and DPP. The lactam groups (C=O) in PDPP-NT possess the obvious ability of obtaining electronic. In a word, the less the charge transfer amount, the smaller the dihedral angle, the better the planarity.

KEYWORDS: D/A copolymer, first-principles, optical absorption, effective mass, Bader charge analysis

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M-P058

专题代号：M

Unusual tribology behaviors of Ferroelectric two-dimensional In_2Se_3 material

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ABSTRACT: Friction is present in almost all moving parts of mechanical systems, and it is often the main cause of energy loss, mechanical failure and inefficiency. In the nanoscale, the friction behavior is usually significantly different from that in the macroscopic regime. Numerous studies have shown that the friction coefficients between two sliding bodies are usually strongly sensitive to a variety of factors, such as external loads, contact areas, temperature, velocity, thickness, and surface topography. However, establishing applicable method in dramatically lowering the friction coefficient in nanoscale is of great challenge. Here, based on first-principles calculations within density functional theory, we explored the effect of ferroelectricity on the friction of the interface of two layers of 2D In_2Se_3, which exhibits room-temperature ferroelectricity with spontaneous electric polarization in both out-of-plane and in-plane orientations. During the sliding process, we investigate the behavior of the friction under different polarization magnitude realized by loading different pressure on the surface of the In_2Se_3 in consideration of two situations, i.e., with the two layers of In_2Se_3 coupled with each other in the same polarization direction (type-I) and opposite polarization directions (type-II), respectively. We find that the band structure of the former exhibits metallic and the latter semi-conductive, respectively. Importantly, we were surprised to find that negative friction occurs in type-II structure, i.e., at the load below 2.75 GPa.

Key words: ferroelectricity，tribology，negative friction.

M-P059

专题代号：M

First-principles Calculations on the Catalytic Properties of Fe Single Atom Stabilized on Honeycomb Borene/Al(111)

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ABSTRACT: 近年来，将金属原子沉积在二维材料上作为高效的单原子催化剂一直处于一个比较热门的研究领域。本文通过采用基于密度泛函理论的第一性原理计将一些单原子金属（其电负性均小于硼）如:Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Cu,Zn 沉积在蜂窝状硼烯/Al(111)衬底上, 金属原子和衬底之间的电荷转移可以使蜂窝状硼烯更加稳定，同时增强金属原子与其成键作用，从而有利于形成高度分散的单原子。比如，单原子 Fe 可以优先沉积于蜂窝状硼烯/Al(111)的中空位上并表现出较高的稳定性。我们进一步模拟了 CO 在 Fe 单原子催化剂上氧化的动力学过程，在 Eley Rideal (ER) and Langmuir Hinshelwood (LH)这两种机制下均表现出较低的反应势垒（分别为 0.62eV 和 0.7eV）。这表明单原子 Fe 所构筑的单原子催化剂体系对 CO 的氧化反应表现出较高的催化活性。我们的研究结果为制备高效、稳定、低成本的单原子催化剂提供了有益的理论借鉴。

Key words: Single atom catalyst; Charge transfer, CO oxidation, First-principles calculation.

M-P060

专题代号：M

通过高次谐波来区分 4 种 MoS₂的晶体相

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摘要：众所周知，晶体对称性影响高次谐波产生。比如，当空间反演对称性破缺时，就会导致偶次谐波出现。对于不同的材料来说，经常会出现各种各样的相。这些相在实验上混淆在一起很难区分，导致材料的性质很难判断。比如，二维过渡金属硫化物（MoS_2）。单层 MoS_2 具有四个主要晶相：1H，1T，1T'和 $1T^d$，其中 1T 与 1T'晶体结构是十分类似的，但是在电子结构上却具有很大的差异[1]。在这里，我们证明 HHG 可以区分 MoS_2 的晶相。当在平面内施加线性偏振光时，观察到来自 MoS_2 的 HHG 具有面内各向异性。因此在线性激光下产生的高次谐波可以用来判断晶体取向。当激光是圆极化时，1H-MoS_2 中的谐波次数为 3n±1；在 1T-MoS_2 中，相比较 1H-MoS_2 中的高次谐波，只有偶次谐波消失而其他阶次保持不变；1T'-MoS_2 仅出现奇数次谐波；在 $1T^d$-MoS_2 中，偶数次和奇数次谐波共同出现。正是晶体对称性和激光极化之间的相互作用导致了高次谐波信号变化。我们的发现不受 Berry 曲率，带内电流和带间极化的影响[2]。我们的研究打开了高次谐波在区分晶体相中的研究，这为以后的实际应用提供了一定的帮助。

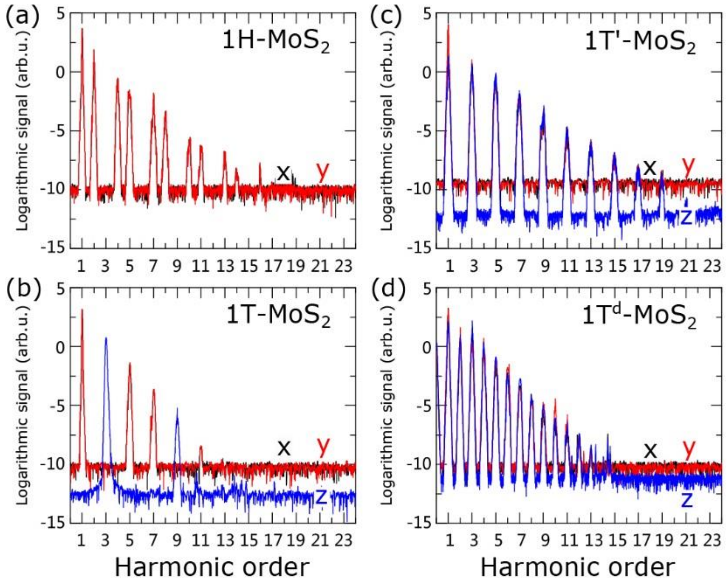

图 1：四种相在圆极化光下的高次谐波。我们能看到这几种相的所产生的高次谐波具有明显的区别，因此圆极化光下的高次谐波用来区分这几种相是很轻松了。

关键字：高次谐波，MoS_2，晶相区分

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M-P061

专题代号：M

Tunable Broadband Hyperbolic Light Dispersion in Metal Diborides

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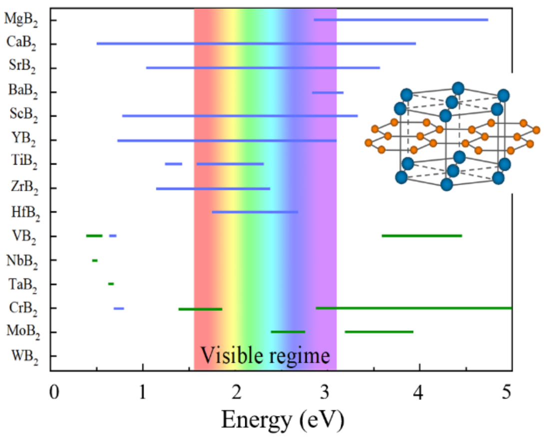
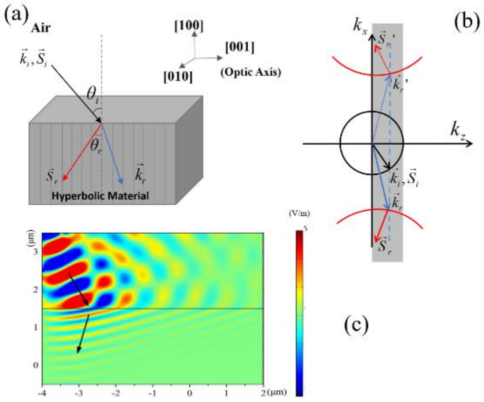
Abstract:The naturally hyperbolic materials that conquer the limitations of artificially structured hyperbolic metamaterials are promising candidates for the emerging devices based on light. However, the variety of naturally hyperbolic materials and their hyperbolic frequency regime reported presently are very limited. Here, on the basis of first-principles calculations, we demonstrated a family of naturally hyperbolic materials, graphite-like metal diborides, with a broadband hyperbolic region from near-IR (~2.5μm) to the ultraviolet regime (~248

nm). The operating hyperbolic window and negative refraction can be effectively modulated by extracting electrons from the materials, offering a promising strategy for regulating the optical properties.





Key： hyperbolic materials; hyperbolic dispersion;all angle refraction effect

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M-P062

专题代号：M

First-Principles Study on the Structure and Magnetic Properties of Two-Dimensional Ferrite

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ABSTRACT: The unique magnetic properties of two-dimensional ferromagnetic materials have important applications in new magneto-optical and magnetoelectric devices such as magnetoresistive memories and spin field effect transistors. Recent studies have shown that the non-van der Waals material Ferrite, which has been stripped from α-Fe_2O_3, is ferromagnetic ordering at room temperature, however its specific atomic structure has not yet been unambiguously determined. In this work, the CALYPSO structure prediction method combined with the first-principles calculations based on density functional theory have been used to establish the geometric structure. It is found that the 1T phase is the ground state of ferromagnetic two-dimensional FeO_2 in consideration of the on-site Coulomb interactions. The Monte Carlo calculation of the Heisenberg model by fitting the parameters shows that the phase transition temperature of 1T-FeO_2 is higher than room temperature. Therefore it may be the most possible stable structure of Hematene. The band structure calculations also show that the 1T-FeO_2 is highly spin-polarized, exhibiting half-metal feature.

Key words: Two-dimensional ferromagnetic, Curie temperature, Hematene.

M-P063

专题代号：M

Molybdenum selenide type nanowires as efficient catalyst for bi-functional oxygen evolution/reduction reactions

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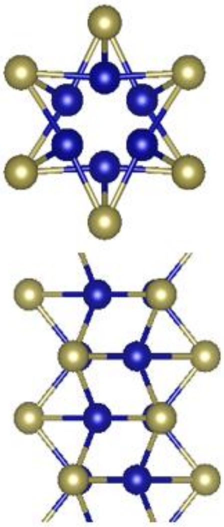
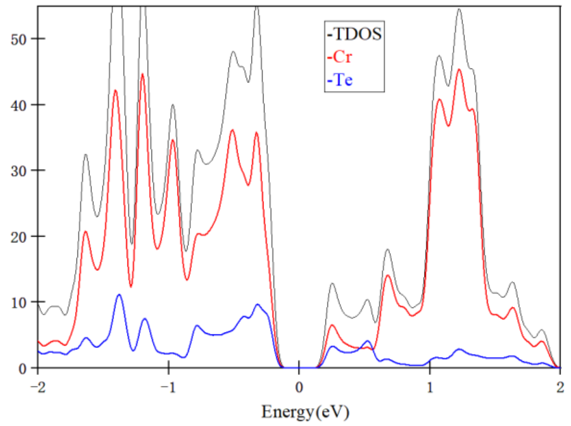
Abstract: The identification of stable bifunctional electrocatalysts for the oxygen reduction and evolution reaction (ORR/OER) is fatal for electrocatalytic water cycle. To our knowledge, the application of nanowires to bifunctional catalyst has been rarely explored. On the basis of first-principles calculations, we systemically investigate Y6X6 (X=S,Se,Te; and Y=Cr,Mo,W)nanowires. Our calculations showed that Cr6Te6 nanowires can serve as efficient OER/ORR electrocatalysts with the overpotentials even lower than the precious-metal-group catalysts. The catalysts ability of nanowires is visibly superior to their corresponding 2D materials, which shows the unique structure of nanowire is beneficial to their catalysts application. To well describe the electrocatalytic performance of candidates, we established a scaling relationship between the adsorption free energies of adsorbates and its overpotential. Our findings offer the promising alternative with the feature of stable, low-cost, and efficient for commercial precious catalysts.





Key: nanowire; bifunctional electrocatalysts ; first-principles calculations

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M-P064

专题代号：M

工业畸变下 Ruby 晶格狄拉克锥的鲁棒性

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摘要：Ruby 晶格由于其奇异的能带结构和拓扑特性，近年来得到了广泛的报道。然而，此类材料在实验制备上的难点之一在于晶格由于制备环境复杂而产生的一定程度的错配和缺陷等工业畸变，而对称性的破坏可能会导致一些重要性质的缺失。

本文讨论了三种简单的畸变晶格，并利用紧束缚近似得到了它们的基本能带性质。结果表明，在 Ruby 晶格与小幅度畸变晶格之间可以实现哈密顿量的幺正变换，并且晶格的大部分重要的性质在形变

中被保留了下来，证明了 Ruby 晶格狄拉克锥对单一对称破坏的鲁棒性。同时，规则的对称性破缺表明，Ruby 晶格的大部分拓扑性质可以在单一对称性存在的情况下得到保留。当两种对称都被打破时，晶格的所有狄拉克锥都消失了。为了印证上述观点，我们利用光子晶格实现了 Ruby 畸变晶格的能带再现，基本能带特点与紧束缚计算结果相吻合，确保了该模型在实验上的可行性。我们的工作证明了 Ruby 晶格狄拉克锥的鲁棒性，拓宽了类红宝石晶格的制备条件，使这种材料更易于在实验上实现。

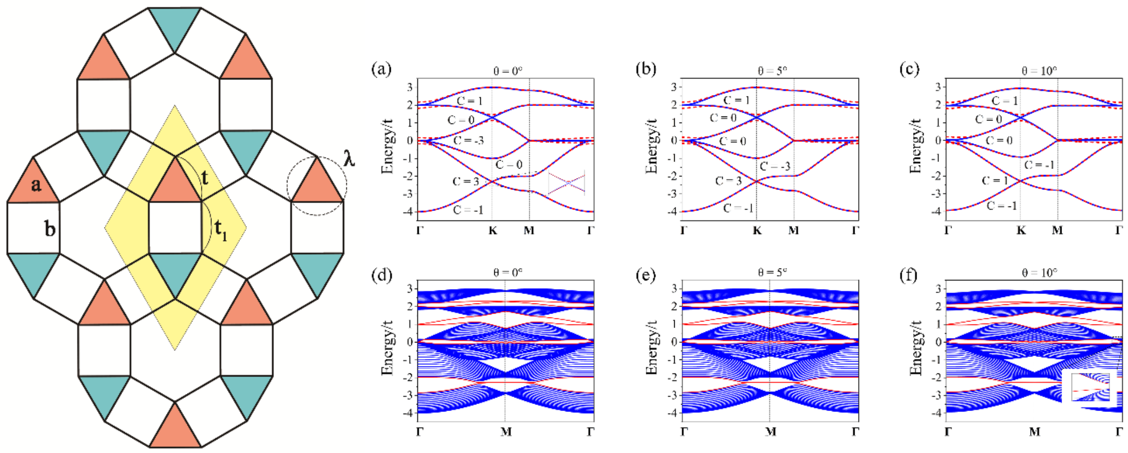

图 1 Ruby 晶格模型与畸变晶格的紧束缚能带和边界态

关键词：Ruby 晶格、紧束缚近似、狄拉克锥

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M-P065

过渡金属修饰手性边缘石墨烯纳米带磁性的第一性原理研究

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摘要：具有手性边缘的石墨烯纳米（cGNR）带两个边缘均呈反铁磁耦合，过渡金属修饰是引入强磁性的有效方法。在实验中也是可行的，如可将 TM 金属原子对单层或双层石墨烯进行替位掺杂。然而，此方法不能精确控制过渡金属掺入的位置。通过自下而上的分子方法，在金属表面对分子前驱体自组装，可以获得原子位置精确的石墨烯纳米带[1-4]。同样，以掺有过渡金属的分子作为前驱体，通过自组装方法，可以得到掺杂位置精确的石墨烯纳米带。基于密度泛函理论，我们研究了过渡金属（Fe, Co, Ni, Cu, Zn）对类 Mpry 分子[5]合成的手性石墨烯纳米带（TM-cGNR)磁性的影响，其结构如图 1 所示。计算结果表明，过渡金属原子掺杂的所有手性石墨烯纳米带都是半导体。Fe 修饰的手性纳米带

(Fe-cGNR)具有铁磁性基态。Fe-cGNR 的能带结构以及磁性基态可以通过载流子掺杂浓度来调节，当载流子掺杂到 0.02 空穴/原子时，其基态由铁磁性转变为反铁磁性。较大的磁各向异性能(190μeV / Fe 原子)也表明该体系具有稳定的长程有序的磁矩。在 4%的轴向拉应力作用下，Fe-cGNR 从铁磁态转变为反铁磁态。我们的研究将有助于进一步研究石墨烯纳米带的自旋控制。

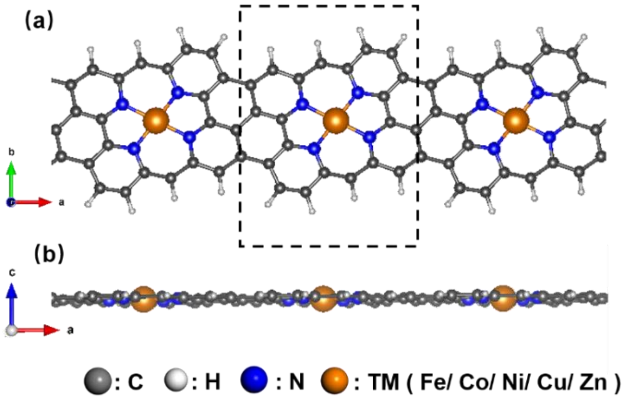

图 1 结构优化后的 TM 原子修饰的手性石墨烯纳米带俯视(a)和侧视图(b)，其中原胞用黑色虚线标记。a、b 和 c 方向分别对应于 x、y 和 z 轴。

关键词：石墨烯纳米带 手性边缘 过渡金属 铁磁性

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M-P066

专题代号：M

二维铁电材料 Sc2P2Se6 及磁性掺杂诱发的多铁性

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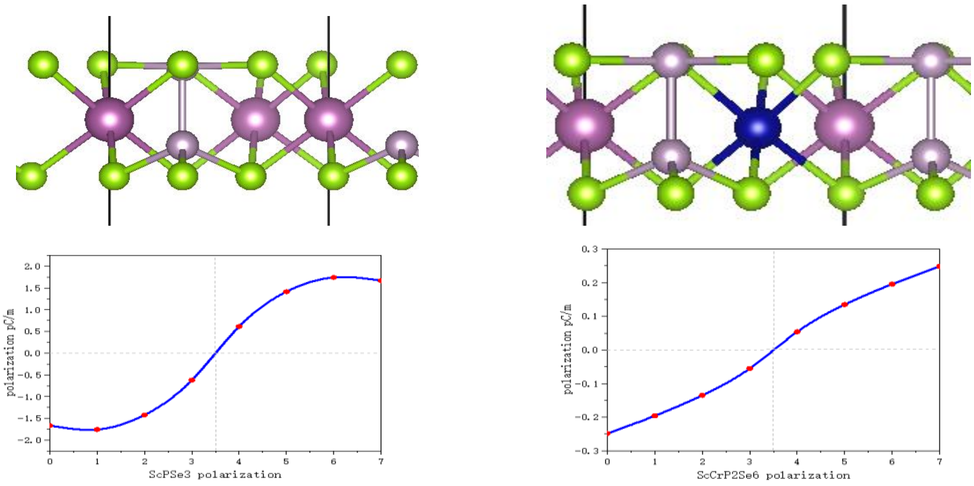
摘要：铁电材料以及多铁质材料具有应用于新型磁电器件的潜力，如高密度非挥发性存储器件。近几十年来，铁电和多铁材料的研究主要集中在三维材料上。然而，三维材料在纳米尺度薄膜中存在悬空键和

量子隧穿现象。二维(2D)材料可能为这些问题提供一种优雅的解决方案，因此需求量很大并可能得到广泛的应用。利用第一性原理计算，预测了二维材料 Sc2P2Se6 单分子层的面外铁电性以及掺杂 Cr 原子的 ScCrP2Se6 单分子层反铁磁性和电场驱动铁电性。在这些单层材料中，磷原子的中心位置远离中心原子平面，沿平面法向产生非平凡的电偶极矩。我们预测 Sc2P2Se6 结构的铁电性在室温下是稳定的。ScCrP2Se6 单层铁电相的总能量要高于反铁电相，使得铁电相处于亚稳态，但铁电相可以通过施加较大的电场来实现。计算结果表明，铁电相具有反铁磁基态，而能量更低的反铁电相具有铁磁基态。它们的面外铁电性表明了利用外部垂直电场控制电极化的可能性，我们的发现可能为进一步的设备应用提供一系列二维材料，用于实现二维纳米级开关和电极存储设备。



Sc2P2Se6 和 ScCrP2Se6 结构以及铁电极化强度

关键词：二维材料　多铁性

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M-P067

专题代号：M

Tunable electronic properties of 2D a-tellurene-based bilayer and trilayer heterostructures

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摘要：Alpha-tellurene (α-Te), a recently theoretically and experimentally accessible Group-VI two-dimensional (2D) material, has attracted considerable attention. Owing to its unique structure being similar to that of 2D transition metal dichalcogenides (TMDs), the studies of 2D van der Waals heterostructures (vdWHs) based on a-Te/TMDs will be very interesting. In this work, we designed the bilayer a-Te/MoS_2 vdWH, trilayer WS_2/a-Te/MoS_2 and a-Te/WS_2/MoS_2 vdWHs, and investigated the electronic properties by using the first-principles method. Our results have suggested that these vdWHs possess an obvious type-I band alignment with an indirect band gap value, which is similar to the monolayer a-Te. Moreover, we have also found that an intriguing type-I to type-II or indirect to direct transition can be induced by increasing the interlayer coupling of the heterostructure or applying the biaxial strain and external electric field. Overall, these findings provide a promising route to tune the electronic properties and design new a-Te-based vdWHs for applications in electronic and optoelectronic devices.

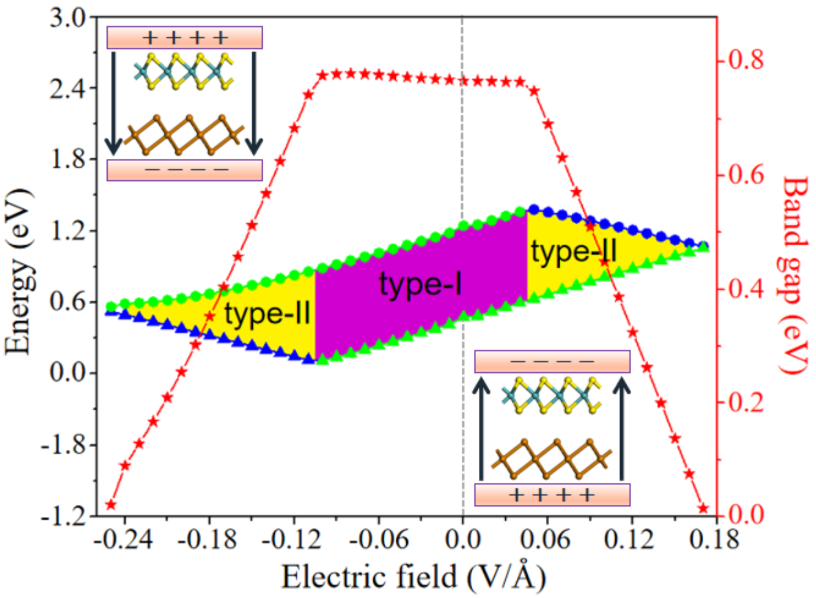

Fig. 1 Schematic diagram of the band edge positions and gap values as a function of external electric field

关键词：a-tellurene heterostructure electronic properties

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M-P068

专题代号：M

铁电极化对 X_3GeTe_2/In_2Se_3 (X=Fe, Mn, Ni)异质结磁性的调控研究

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摘要：对多铁材料的磁性进行有效调控不仅在科学上具有重大意义，在现代工业上也有紧迫需求。然而，单相多铁材料不但种类少而且磁电耦合较弱。人们通常把关注重点放在由铁磁材料和铁电体构成的异质结或超晶格体系中。二维(2D)范德瓦尔斯材料，例如 CrI_3，$Cr_2Ge_2Te_6$和 Fe_3GeTe_2等，由于具有优异的性质近年来得到了人们的广泛关注。本文采用第一性原理方法，从原子尺度上设计了三种沿着(001)晶向并含有 15 埃的真空层的异质结，即 Fe_3GeTe_2/In_2Se_3 (FGT), Mn_3GeTe_2/In_2Se_3 (MGT)和 Ni_3GeTe_2/In_2Se_3 (NGT)。通过铁电极化成功实现了三种异质结的磁性调控。结果表明，铁电极化可以同时或者单独控制原子的磁矩，磁序，电导率和磁交换作用。铁电极化破坏了体系的对称性，导致界面附近的磁性原子的 3d 轨道出现了电子转移和化学键重构，这可能是体系磁性能够被调控的原因。本文研究发现可以通过铁电极化有效调控异质结的磁性并实现强磁电耦合。我们构建的模型是一种有较高科学价值的模型，可以为将来的 2D 范德瓦尔斯磁性材料领域的研究提供指导。

关键词：第一性原理；多铁性；磁性；铁电极化

Keywords：First-principles; Multi-ferroelectric; Magnetism; Ferroelectric polarization

M-P069

专题代号：M

第一性原理研究 Co2FeAl/MgO/Co2FeAl 多层材料的与磁相关的塞贝克效应

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摘要： 由于新奇的物理特性和在自旋电子学中的潜在应用，与磁相关的塞贝克效应已经获得了人们的广泛关注。本文我们采用第一性原理计算和自旋分解的玻尔兹曼输运理论，系统的调查了两种界面终端(Co_2/O 和 FeAl/O 终端)在磁态平行和反平行的条件下 $Co_2FeAl/MgO/Co_2FeAl$ 多层的电子结构和自旋相关的输运性能。我们的结果指出 Co_2/O 终端的与磁相关的塞贝克效应是和实验值更一致的。此外，对于 Co_2/O 终端界面，无论是平行态还是反平行态，相应的自旋塞贝克值都大于较好的 $Co_2MnSi/MgO/Co_2MnSi$ 异质结构。而这种现象只发生在 FeAl/O 终端的反平行态。 为了更深入的分析上述结果的产生原因，我们研究了两种不同终端的几何结构、电子结构、磁行为的差异性。结果，我们发现两种终端在界面区形成反键和成键态、重调了能隙值、改变了 O 原子的磁动量、提升相应的自旋极化值到-82%等。这些现象是导致上述结果产生的原因。同时，这些变化也伴随着界面区 Co/Fe 3d 电子态和 O 2p 电子态的相互杂化和电荷转移作用。导致了在远离界面区电荷密度呈现奇异的形状，比如，Co_2/O 终端的 Co 原子形成了蝴蝶结形状的电荷密度，而 FeAl/O 终端的 Co 原子形成了脚丫形状的电荷密度。 此外，Co_2/O 终端界面形成了自旋劈裂的输运带隙伴随着半导体输运性质，而 FeAl/O 终端的带隙则关闭并展示了金属特性。我们的发现将对实验上设计与磁相关的塞贝克设备有进步性的指导意义。

关键词：第一性原理；玻尔兹曼输运；塞贝克效应；输运性能

基金项目：国家自然科学基金项目（N0s. 11674083， 21603056， 11305046）河南省基金 （Nos. 182106000023，182102410096，and 182300410227）.

M-P070

专题代号：M

稀土铁氧体 AFeo3（A=Lu，Y，和 Gd）中磁畴壁诱导铁电极化的第一性原理研究

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摘要：第 II 类多铁体的铁电性是由特定的磁序引起的；由于具有极大的磁电耦合以及在信息存储，电子和传感器中巨大的潜在应用价值，使得第 II 类多铁体成为最激动人心的材料之一。由于自旋序不连续能够提供可能的自旋阻挫，使得畴壁成为一个理想的平台来研究畴壁上相关的物理性质。本文通过第一性原理计算，结合对八面体形变和统一极化模型的分析，计算了稀土正铁氧体铁氧体 $AFeO_3$（A = Lu，Y，和 Gd）中反铁磁畴壁诱发的铁电极化。我们发现，稀土正铁氧体中 A 位元素对铁电极化的大小具有不可忽视的影响：A 位元素的离子半径越小，在最大的畴壁密度情况下，其相应的化合物的极化值越高，最大的铁电极化（0.092 uC / cm^2）出现在 $LuFeO_3$ 有着最大畴壁密度的构型中。为了进一步理解铁电位移的起源，我们从结构角度分析了阴阳离子位移，直观的阐述了极化出现的方向。同时发现，畴壁处氧八面体的倾斜是造成诱导极化产生的主要原因。对于这三种物质，八面体倾斜角的变化量满足 $LuFeO_3 > YFeO_3 > GdFeO_3$，因此，他们在畴壁处诱导的极化值将满足 $LuFeO_3 > YFeO_3 > GdFeO_3$，符合半径的依赖关系。此外，通过统一极化模型，我们再次解释了正铁氧体畴壁上的铁电极化沿 b 方向的原因，并对反铁磁畴壁上铁电性的微观起源进行了详细的阐述，对 $LuFeO_3$、$YFeO_3$、$GdFeO_3$ 的微观上极化值的差异性进行了定量分析。研究发现：不同的八面体倾斜角和不同的晶胞体积是导致三种化合物极化差异的主要原因。我们的研究为磁畴壁上 II 型多铁体的实验设计提供了坚实的理论支持。研究结果提高了对畴壁磁诱导铁电极化的理论认识，并为基于畴壁多铁性的自旋电子器件的实验应用提供了依据。

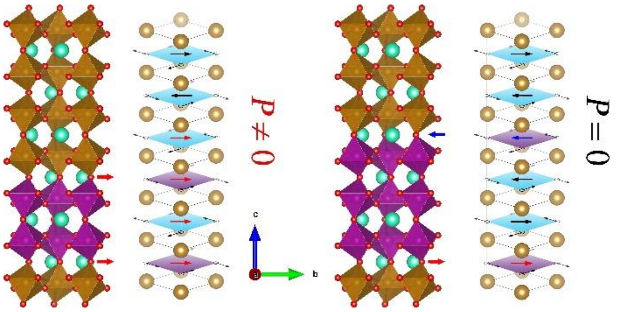

FIG.1 The spin-induced ferroelectric polarization at the magnetic domain walls is dependent on the A-site ionic radius of $AFeO_3$.

关键词：第一性原理计算，多铁，磁畴壁，铁电极化

基金项目：国家自然科学基金项目（(No. 51571083 和 11674083)

M-P071

专题代号：M

钙钛矿氧化物异质结中极化对磁性的调控

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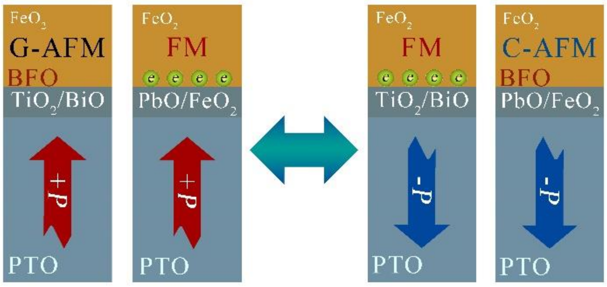
摘要：随着信息技术的迅速发展，具有磁电耦合的多铁材料已经成为高密度非易失性随机存储器，传感器和其他微电子领域应用的最有希望的候选材料。然而，自然界中室温单相多铁材料十分稀少。为此，基于钙钛矿氧化物异质结的人造多铁材料最近引起了人们极大的关注。

在这项工作中，我们不仅展示了极性钙钛矿氧化物界面的丰富物理性质，而且还可以通过切换 PbTiO3 /四方 BiFeO3（BFO）铁电异质结中的极化来调整这些性质。第一性原理计算表明，磁性和导电性可以通过界面处极化不连续和化学价不连续的共同作用引起，并且通过极化的反转，异质结的一些特性也受到了稳健地操纵。这些特性包括界面二维电子气和磁性之间的耦合，从半金属到带绝缘体或 Mott 绝缘体的过渡，以及从 G 型反铁磁到局部铁磁，最后到局部 C 型反铁磁的转换。此外，通过设置不同的终端，我们可以人为地控制在任何一个极化方向上发生的局部铁磁序，甚至可以控制局部铁磁序是出现在界面还是表面。这种新颖的控制可以被应用于存储器件的制造中，它将实现电场写入（切换铁电极化）同时磁性读取的方式进行信息存储，从而大大降低能耗。



关键词：第一性原理计算　钙钛矿氧化物异质结 界面多铁

基金项目：国家自然科学基金项目（(No. 51571083 和 11674083)

M-P072

专题代号：M

Li_6P 电子化合物超导电性的理论研究

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寻找高温超导体是凝聚态物理领域的重要研究课题[1-2]。电子化合物中部分电子聚集在晶格间隙，充当阴离子角色，这些间隙电子在很大程度上决定了化合物的物理性质。由于强电子局域，电子化合物通常为绝缘体。但最近实验发现了一个有代表性的电子化合物$[Ca_{24}Al_{28}O_{64}]^{4+}(e^-)_4$具有超导性（超导转变温度为~0.4 K）。这一发现开创了超导体研究的一个新种类，为超导研究领域注入新的力量。碱金属和碱土金属在高压下容易失去 s 轨道电子，形成电子化合物。考虑到磷元素适中的电负性和超导电性，在富锂组分 Li-P 化合物中磷会捕获一部分电子，剩余电子可能存留在间隙中。由此，通过调控化合物中锂磷比例有望调节间隙电子形态，进而得到具有新奇电子性质的化合物。通过第一性原理的群体智能结构计算发现 Li_6P 电子化合物，超导转变温度高达 39.3 K，刷新了现有电子化合物的记录[1]。间隙电子对 Li_6P 超导性起到重要贡献。

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M-P073

专题代号：M

典型功能材料的高压理论设计

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摘要：能源、超硬、超导等功能材料在新能源开发、高精密机械加工、地质钻探、石油开采、磁悬浮等方面存在广泛的应用。利用高温高压等极端条件制备新材料和高压方法获得高压相材料多功能超硬材料发展的相辅相成的两个重要方面，也是当前国际上凝聚态物理研究的热点，而高压合成是设计、发现

新材料的必要手段。利用 CALYPSO 结构预测方法，系统探索了典型氢化物超导、高能密度材料以及超硬材料等功能材料的高压相图，并分析了其功能特性与其结构电子性质之间的关系，为功能为导向的材料设计的设计提供了理论依据。

关键词：第一性原理，功能材料，高压

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基金项目：国家自然科学基金项目（N0. 11774140）

M-P074

Chirality dependent dielectricity in Moiré antiferromagnet

Yu-Hao Shen, Wen-Yi Tong, He Hu, Jun-Ding Zheng, Chun-Gang Duan

Twistronics rooted in the twisted bilayer van der Waals crystals has attracted immense attention. It demonstrates the interlayer twist giving rise to patterned interlayer coupling which significantly modulates the correlated electronic behaviors. Of particular interest is the 30° twist in the honeycomb bilayer system, which possesses an incommensurate Moiré pattern. A tiny rotation will result in a commensurate superlattice, indicating the system is extremely sensitive to further twist and many intriguing phenomena will occur.

For transition-metal dichalcogenides (TMD) bilayers, there generates two different stackings (H-type like and R-type like) for the case of relative left or right twist from 30°. It is found that a giant dielectric difference of these two stacking cases appears with an interlayer bias applied. In this Letter, we report an exotic dielectric difference in twisted magnetic TMD bilayer systems by *ab-initio* calculations. It would be exciting to realize that chirality dependent twist shows amplified or suppressed dielectric response. Using a two-band model Hamiltonian with both a pseudomagnetic field and vertical electric field considered, the physical mechanism is illuminated. Here, we show a distinct magnetoelectric effect, responsible for the none dipole induced in the right twisted case, where there only induces the spirally redistribution of the planar charge, and a ***negative*** dipole induced in the left twisted case, where the system exhibits strong resistance to the vertical electric field. It is demonstrated this unique dielectricity belongs to the Moire antiferromagnet, which possess intralayer ferromagnetic coupling and interlayer antiferromagnetic coupling.

Practically, we point out that by means of the selective circularly polarized optical absorption, the two chirality dependent Moiré patterns can be distinguished. Our findings enrich our understanding of electron correlation behaviors with the introduction of magnetic ordering to the twisted bilayers and open an appealing route toward functional 2D materials design for electronic and optical devices.

M-P075

专题代号：M

有机光电器件内非均匀电场驱动的激发态超快输运

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摘要：在有机器件中，激发态（如激子和双激子）的输运对于它们的功能过程至关重要。 在这个工作里，通过将局部非均匀电场应用于有机聚合物，我们从理论上提出了一种新的策略来控制激子和双激子的定向和超快输运。 特别是，我们发现双激子的输运方向与激子相反。其基本机制归因于激子和双激子的反向极化行为导致产生相反方向的驱动力。 基于这些发现，我们以有机发光为例，设计了一个有机发光器件的光电调制方案，旨在通过控制其定向输运来实现激子或双激子在有机发光层中的超快重分布。 最后，我们进一步讨论了响应时间和分辨率范围对于发光调制在实际应用中的影响。

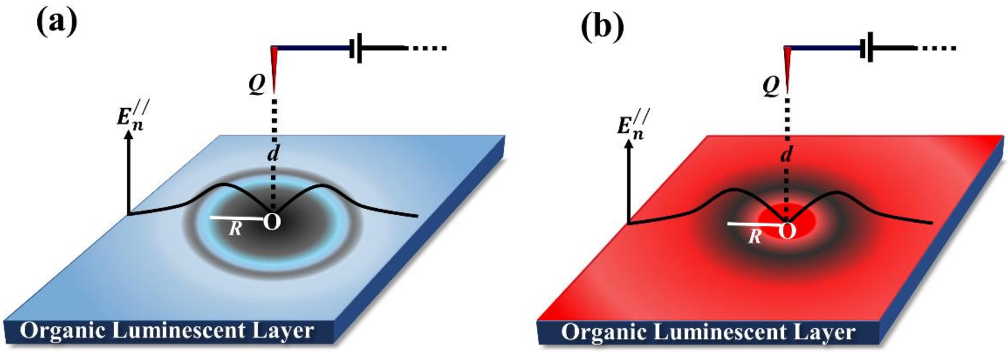

图 1. 操纵激子(a)和双激子(b)的输运方向来调制有机发光的设计方案示意图。非均匀电场的产生是通过在有机发光层上使用带电探针。黑色曲线表示沿单个聚合物链的非均匀电场分布。

关键词：有机器件，光电调制，激子和双激子，定向输运，非均匀电场

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国家自然科学基金 (Nos. 11674195, 61874068)

M-P076

专题代号：M

Mg 掺杂 $LiBH_4$ 与 $Li_2B_{12}H_{12}$ 放氢性能的第一性原理研究

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摘要：近年来，金属硼氢化物复合体系 $LiBH_4$-MgH_2，由于储氢容量高（~11.4 wt%）、可逆储氢性能良好，倍受研究学者关注。对于 $LiBH_4$-MgH_2 复合体系的脱氢反应，尽管实验提出不同方式（如式 1-3），但一致认为脱氢产物 MgB_2 生成对促进体系脱氢起到关键作用，而且 $LiBH_4$ 自分解中间产物 $Li_2B_{12}H_{12}$ 存在会阻碍脱氢产物 MgB_2 生成，由此导致 $LiBH_4$-MgH_2 体系放氢能力下降。

$$2LiBH_4+MgH_2\rightarrow 2LiBH_4+Mg+H_2\rightarrow MgB_2+2LiH+4H_2 \tag{1}$$

$$12LiBH_4+6MgH_2\rightarrow Li_2B_{12}H_{12}+10LiH+6MgH_2+13H_2\rightarrow 6MgB_2+12LiH+24H_2 \tag{2}$$

$$12LiBH_4+6MgH_2\rightarrow Li_2B_{12}H_{12}+10LiH+6MgH_2+13H_2\rightarrow Li_2B_{12}H_{12}+10LiH+6Mg+19H_2\rightarrow 6MgB_2+12LiH+24H_2 \tag{3}$$

为了解 $LiBH_4$-MgH_2 体系的放氢机制，尤其是 $LiBH_4$ 自分解中间产物 $Li_2B_{12}H_{12}$ 在体系脱氢过程的作用，研究基于上述 $LiBH_4$-MgH_2 脱氢反应的两种方式 $LiBH_4$+Mg 和 $Li_2B_{12}H_{12}$+Mg，采用第一性原理构建 Mg 掺杂 $LiBH_4$-Mg 和 $Li_2B_{12}H_{12}$-Mg 体系，对比分析两掺杂体系的脱氢性能和电子结构。研究结果表明，尽管 Mg 掺杂均有效提高 $LiBH_4$ 和 $Li_2B_{12}H_{12}$ 的放氢性能，但与 $LiBH_4$-Mg 体系相比，（1）$Li_2B_{12}H_{12}$-Mg 体系氢解离能较高，脱氢能力较弱，原因是该体系 B-H、Li-B/H 作用较强，而且其脱氢过程会抑制 MgB_2 生成；（2）$Li_2B_{12}H_{12}$-Mg 强烈的 B-B 作用不利体系可逆储氢，因为强烈的 B-B 作用被认为是阻碍金属硼氢化物脱氢中间产物 $M_2B_{12}H_{12}$ 可逆储氢的主要因素。由此研究认为，为提高 $LiBH_4$-MgH_2 体系的储氢性能，其脱氢过程应抑制 $LiBH_4$ 自分解中间产物 $Li_2B_{12}H_{12}$ 的生成，该结论与实验报道观点一致。

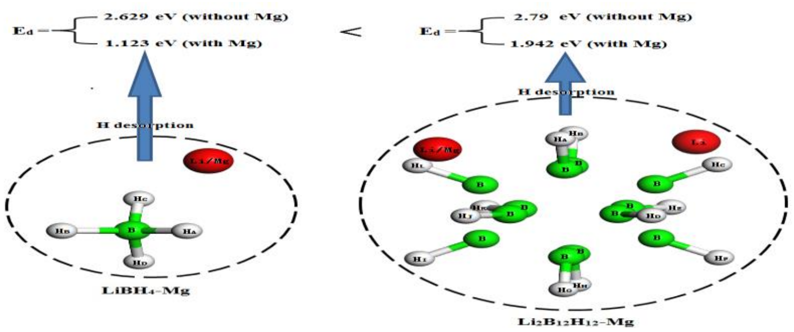

图 1 $LiBH_4$-Mg 和 $Li_2B_{12}H_{12}$-Mg 体系的放氢性能

关键词：$LiBH_4$ $Li_2B_{12}H_{12}$ Mg 掺杂 第一性原理计算 放氢性能

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M-P077

专题代号：M

有机聚合物中交换耦合作用诱导的自旋输运

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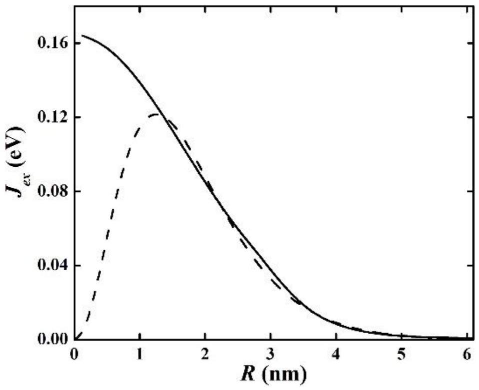
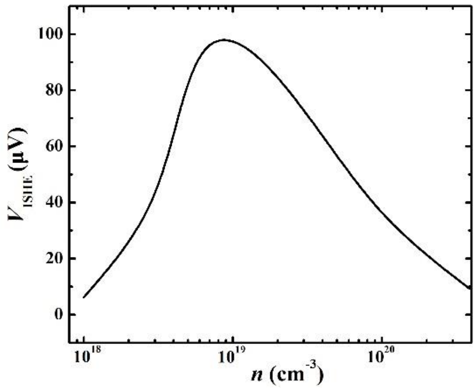
摘要：自旋泵浦产生的纯自旋流在有机半导体中输运的实现，激发了对有机半导体中自旋输运机制的研究。然而目前为止，关于自旋输运机制的讨论依然充满争论。在本篇文章中，我们系统地阐述了有机半导体中自旋交换耦合作用诱导的自旋输运。利用 SSH 模型，我们计算了自旋的注入和输运，及极化子之间的交换耦合强度与杂质浓度的关系。此外，我们基于极化子间的交换耦合机制提出了自旋输运的速率方程，并计算得到了与实验结果相符合的自旋扩散长度和霍尔电压。更有趣的是，我们发现霍尔电压随掺杂浓度的变化是非单调的，通过调节掺杂的浓度可以得到霍尔电压的最大值。我们的研究结果将激励实验工作者在多种掺杂浓度的有机半导体中研究纯自旋流输运。



图一：交换耦合强度随极化子之间的距离的变化(实线)



图二：霍尔电压随杂质浓度的变化

关键词：纯自旋流，自旋输运，有机半导体

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M-P078

专题代号：M

氧族元素对 D-A 共聚物电子结构和光吸收谱影响的第一性原理研究

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摘要：本文基于第一性原理密度泛函理论，首先以氧族元素替换 D-A 共聚物 PBDT-BT 中 D 单元 X 位和 A 单元 Y 位，研究了两种替换方式下该共聚物的电子结构。结果表明：D 单元上 X 位替换前后分子前线轨道变化明显，带隙值依次降低。D 单元上 X 位替换时中心键长随替换原子电负性强弱依次减小。采用 Bader 电荷分析得出 D-A 间的电荷转移量，D 单元 X 位 S 替换时，差分电荷密度图的电荷分布相比于 X=O、Se、Te 有较大的变化。分析认为主要是 S 原子有 3d 空轨道。D 单元 X 位 Se、Te 原子的替换有较高 Bader 电荷交换量，有助有带隙值的降低；A 单元 Y 位替换对于聚合物分子前线轨道及电荷转移量影响均较小。总之，D 单元 X 位氧族元素替换对共聚物分子电子结构影响较大，有助于降低带隙、提高迁移率。

再用噻吩环作为 π 桥，构造出 D-π-A(PBDT-DTBX, X = O, S, Se, Te)结构.系统地计算相应的光吸收谱. 比较不同氧族元素和噻吩 π-键桥对聚合物光吸收谱的影响. 研究结果表明：D-A 共聚体中

当 X 位元素以 O，S，Se，Te 替换时，其体系的最高占有分子轨道(HOMO)能级变化不大，最低未占有分子轨道 (LUMO)能级逐渐靠近费米能级，带隙逐渐减小. 在可见光区有两个较强的吸收峰，随着 X 位元素原子序数增大，位于 4.0 eV 左右的光吸收峰位基本不变，另一光吸收峰强度明显增大并发生红移. 与 D-A 结构相比，D-π-A 结构的带隙均有所减小，其中 X 为 Te 时带隙最小；光吸收峰强度随着氧族元素原子序数的增大也明显增大并发生红移. 通过比较光吸收系数和相应态密度，结果表明，4.0 eV 左右的光吸收峰主要是 BDT 单元的贡献，氧族元素的改变主要影响 519.4—703.9 nm 范围的光吸收。

关键词: 密度泛函理论 D-A 共聚物 电子结构 光吸收谱

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M-P079

专题代号：M

键无序对π通量正方晶格基态反铁磁性的影响

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摘要：固体材料有可能以多种方式偏离理想的周期性。例如晶格畸变、杂质原子和晶格缺陷都可能造成这种偏离，这种偏离统称为无序。自从上世纪八十年代发现铜酸盐的铜-氧面的磁性可能在其高温超导机制中起重要作用，人们对无序（尤其是低维淬灭无序）的研究产生极大热情。Nicolas Laflorencie 等人通过数值模拟得到在基态的自旋 1/2 海森堡反铁磁模型上，正方晶格的反铁磁性随无序降低，但只有无穷大的淬灭无序才能破坏系统反铁磁性，其磁长程相互作用十分稳固。由 lan Aflleck 提出的π通量的正方晶格被认为与高 Tc 铜基体的能隙有关，且其与石墨烯同具有狄拉克费米属性，因此得到人们的广泛关注。

本文利用量子蒙特卡罗中随机级数展开的数值方法研究了键无序对 π 通量正方晶格基态反铁磁性的影响。研究发现，随着无序强度的增大，系统反铁磁性减弱，但与理想正方晶格不同的是，π通量正

方晶格反铁磁性不如纯的正方晶格稳健，存在临界的键无序程度使得π通量正方晶格反铁磁性消失。

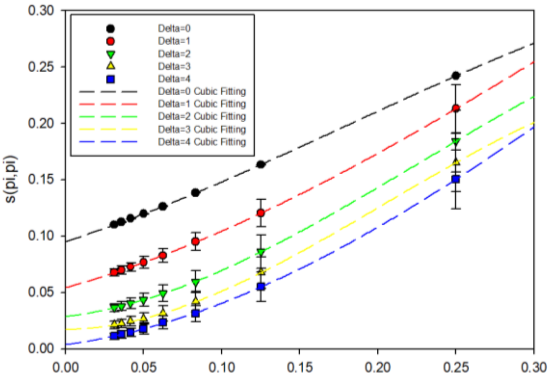

图 1 含π通量的正方晶格在不同无序强度下的反铁磁性随晶格尺度的变化

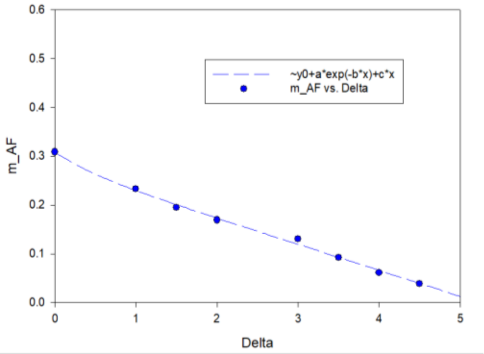

图 2 交错磁通强度对无序强度的拟合

关键词：含π磁通的正方晶格；键无序；反铁磁性；狄拉克费米子

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M-P080

专题代号：M

有机半导体中热诱导激子扩散和解离

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摘要：尽管在过去的几十年中，有机太阳能电池取得了很大进展，与无机太阳能电池相比，有机光伏器件的效率仍然有待提高，因此理解有机光伏过程的物理机制至关重要。由于有机半导体具有强的电-声耦合，导致有机体系中的激子具有很强的束缚能，约 0.2-1.0 eV，而室温热能约为 0.026 eV，从经典统计来看，仅仅依赖室温热能似乎很难将激子解离。然而，近年来，一些实验研究表明，即使在室温下，温度效应的存在对激子扩散或解离也是有效的。此外，在实际器件中由于光照、材料的热容等因素的影响，活性层中的温度分布是非均匀的。为了更深刻的理解温度效应对光伏过程产生的影响，我们引入热效应（π电子按照费米-狄拉克分布、原子核满足玻尔兹曼分布），利用紧束缚模型，我们研究了有机

光伏器件活性层中非均匀温度分布对激子扩散和解离的影响。发现热效应可以使激子中的电子-空穴发生分离，并且随着温度的升高，分离变得明显。特别是，当沿聚合物链施加线性梯度温度分布时，发现激子将沿着链向高温区域移动。基于此，我们提出了一种内建热场驱动激子扩散和离解的物理机制，为提高有机太阳能电池的效率提供了新的有效途径。

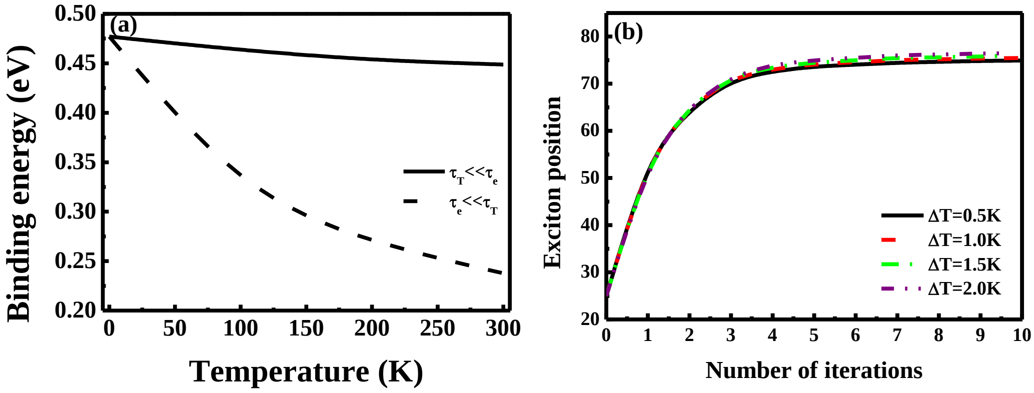

图 1　(a) $\tau_T \ll \tau_e$（实线）和 $\tau_e \ll \tau_T$（虚线）时，激子束缚能随温度的变化

(b) 不同温度梯度下，激子位置的演化

关键词：有机太阳能电池 非均匀热场 激子扩散 激子解离 激子极化

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基金项目：国家自然科学基金项目（N0. 11574180）

M-P081

专题代号：M

网格状单层 MoTe2 的电子结构和磁学性质

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摘要：二维过渡金属硫族化合物（TMDs）有着优异光电特性，目前受到了材料科学领域的广泛关注。之前的实验研究发现，通过 MBE 方法生长的单层 $MoSe_2$ 中会出现三角形网状的畴界。单层 MoS_2 中可以出现不同晶相（半导体性的 2H 相和金属性的 1T 相）共同稳定存在的现象。2017 年，实验上制备出了有着 2H 相与 1T 相以三角网状交替存在的超结构的单层 $PtSe_2$，这种超结构可以实现选择性吸附分子和纳米团簇且有着优异的催化性能。基于之前所做的工作，我们希望在单层 $MoTe_2$ 中尝试类似

结构，以期能实现同样甚至是更好的性能。

本研究使用第一性原理计算了单层 $MoTe_2$ 中 1T 和 2H 相间交替形成的网格状结构。结果表明，体系结构越大，形成能越小，SOC 效应对体系能带结构影响较大。网格状 $MoTe_2$ 单分子层的尺寸诱导磁性产生，且磁性主要来自界面上的 Mo 原子。具有最大磁矩的 Mo 原子位于对称性最低的点，这种局域磁性使此类网格状体系有可能用于磁存储。不同尺寸的系统表现出不同的磁性特点：随着尺寸的逐渐增大，由于 Mo-2 原子 e_1 和 a 轨道的电子结构的改变，系统将由铁磁性转变为反铁磁性。我们的工作对 TMD 薄膜中原子厚度的高度有序结构进行了详细分析，为进一步研究催化和吸附打下基础。

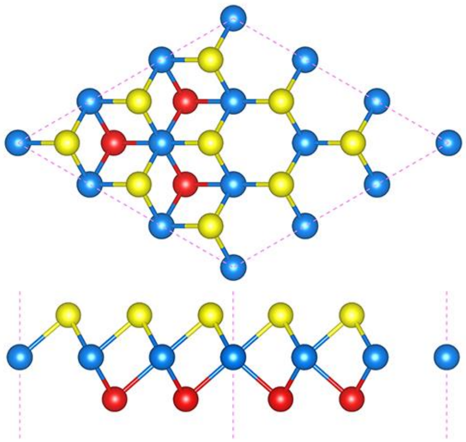

图 1　3×3 网格状单层 $MoTe_2$ 俯视图及侧视图。蓝色、黄色和红色原子表示 Mo 原子、顶层 Te 原子以及底层 Te 原子。

关键词：单层 MoTe2 网格状结构 磁性

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M-P082

专题代号：M

给/受体界面处聚合物非均匀堆叠驱动的电荷转移，弛豫和分离动力学

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摘要：尽管单结和叠层有机太阳能电池的效率在近期都已突破了 15%，但是深入理解给/受体界面处的电荷动力学过程以及相应的能量损耗依然是亟需解决的重要课题。通过模拟由聚合物/富勒烯混合相向聚合物纯净相过渡区处的给/受体界面，我们揭示了激子到达该界面后的电荷动力学过程。发现，对于

给定的聚合物堆叠构型，电荷动力学由给/受体界面处的带阶决定。在小带阶情形下，激子通过电荷转移发生解离，随之形成电荷转移态。当带阶较大时，在聚合物非均匀构型的驱动下，激子可以实现长程的电荷分离，但是必须先经历电荷的转移和弛豫过程。此外，通过计算，我们发现该电荷分离过程的能量损耗由带阶决定。重要的是，我们发现富勒烯的聚集或结晶能够减小激子的束缚能，从而降低该电荷动力学过程中的能量损耗。

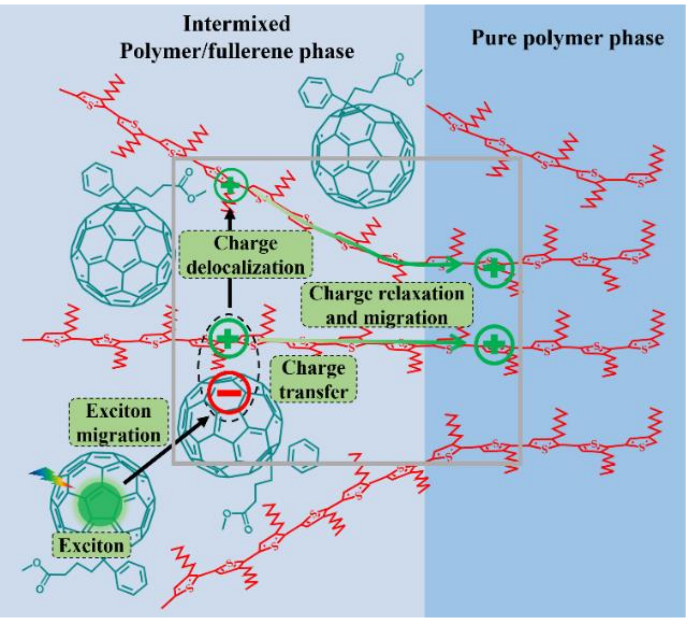

图 1 激子到达给/受体界面后，由非均匀聚合物排列构型驱动的电荷动力学。

关键词：有机太阳能电池 电荷动力学 能量损耗

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M-P083

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新型二维硒化物热电材料的第一性原理研究

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摘要：热电材料能够废热直接转化为有用的电能，对解决能源危机和环境污染具有重要意义。高性能硒

化锡热电材料的发现表明，寻找基于非谐振动效应等因素产生的具有本征低声子热导率的单相热电材料，是提高热电效率的有效途径。基于上述观点，我们提出了一类新的拥有较低本征热导率的二维硒化物（MSe, M=Ge, Sn, Pb），并详细地研究了它们的输运性质。该材料可以看作是在层状化合物 Ge_4Se_3Te [*Angew. Chem. Inter. Edit.*, 2017, 56, 10204]中对锗和碲等价取代而形成的一类新的层状硒化物。理论计算表明，原子层的反平行运动可以导致二维硒化铅材料拥有较强的光声声子耦合效应，低的声子群速度（0.81-2.03 km/s），和较大的格林爱森参数（~4）。在室温下，二维硒化铅展现出很高的塞贝克系数（~1150 μV/K）和极低的导热系数（~0.26 Wm^{-1}K^{-1}）。在 700K p 型掺杂下，二维 GeSe、SnSe 和 PbSe 的热电优值分别为 1.94、2.56 和 5.04。同时我们发现，该类材料的晶格热导率几乎与它们的最低光学声子频率值成正比。这些工作为新型硒化物在热电学的应用提供理论依据，并进一步激励实验对该类化合物展开研究。

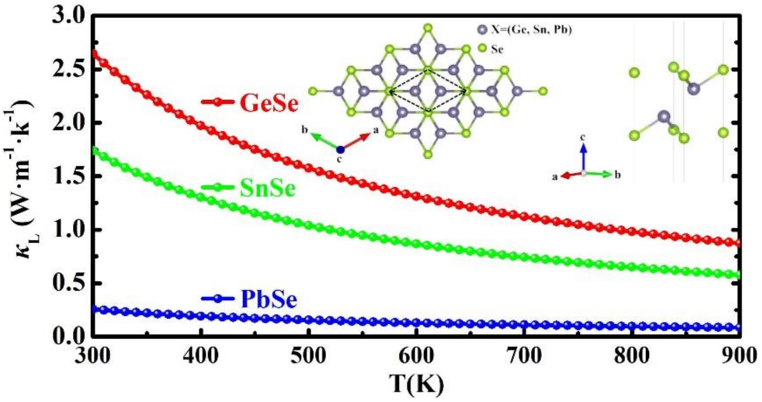

图 1 二维硒化物的结构以及热导率

关键词：热电材料、热导率、电输运、硒化物、第一性原理

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基金项目：广东省自然科学基金博士启动项目（No. 2018A0303100013）

M-P084

专题代号：M

氧气在铀金属表面上分解过程的从头算分子动力学方法的研究

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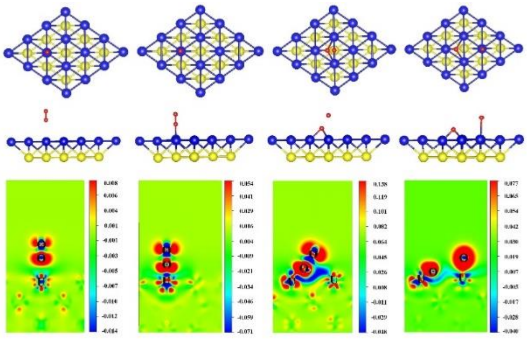
摘要：通过运用从头算分子动力学模拟（AIMD）,本文研究了氧气在 γ-U(110)表面的吸附和分解过程。我们使用了 3×3 的超胞模型，其中（110）方向的铀原子有 5 层，并且真空层的高度为 15 Å。表面模型底 2 层的铀原子被固定了，上 3 层铀原子可以自由驰豫。氧气的初始高度为 3 Å。我们探讨了氧气在四个不同的高对称性点位：顶点位（T）,长桥位（LB）,短桥位（SB）,以及三重空位（3FH）。考虑到氧气在铀表面上不同的排列方式，氧气在 γ-U(110)表面的 8 种吸附情况已经得到了研究。我们发现氧气在靠近表面的过程中会自发的分解。我们重点探讨了其中三种典型的分解路径。如果氧气被放置于 γ-U(110)的顶点位，并且垂直于表面，在进行分子动力学模拟过程中发现，氧气在接近铀表面时，会逐渐发生旋转，最后平行于表面。当氧气被放置于 γ-U(110)长桥位时，无论是平行或是垂直于表面，氧气都会进入到第二层表面中，并且保持为高对称性结构。投影态密度（PDOS）和电荷密度图（CDD）被用来分析氧气的吸附和分解过程。氧气在铀钼金属（110）表面的吸附和分解同样得到了进一步地研究（也就是一个钼原子替换了铀表面上的一个原子），我们同样发现了，氧气会在铀钼表面上自发的分解. 并且，氧气在铀钼表面上的分解速度远远快于纯铀表面。



(a) t=0 fs (b) t=69 fs (c) t=732 fs (d) t=766 fs

图 1 氧气在铀表面上不同时间的轨迹图及相对应的差分电荷图

关键词：γ-U(110)表面 氧气吸附与分解 从头算分子动力学研究

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M-P085

专题代号：M

理论预言顺磁电子晶体 Y_2C 中存在 Weyl 费米子

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摘要：随着实验证实材料中存在Weyl费米子，研究Weyl费米子的物性成为凝聚态物理学的前沿热点之一。 基于密度泛函理论的第一性原理计算，我们发现在二维层状的电子晶体Y2C中存在Weyl费米子。计算结果表明Y原子的4d轨道和层间电子的s轨道发生了杂化，在费米能附近产生了范霍夫奇点，导致了较大的电子态密度，根据Stoner-type判据，得出Y2C倾向出现自旋极化，出现铁磁基态。铁磁的出现，打破了Y2C体系中的时间反演对称性。在不考虑自旋轨道耦合的作用下，体相Y2C中出现了受对旋转对称性称性保护的Weyl nodal lines。自旋轨道耦合作用的出现会使这些nodal lines会转化成Wey费米子，并在表面产生了非平庸的表面态费米弧。同时，我们通过改变磁轴的方向，可以改变Weyl费米子的位置，但是由于Y2C具有非常小的自旋轨道耦合作用，磁轴方向的改变，并不能明显改变表面态。进一步，我们的计算结果表明Y2C中具有非常小的磁各异性能，这与实验观测Y2C单晶在2 K温度下具有顺磁性是一致的。总之，我们通过理论计算预言在二维Y2C电子晶体中存在Weyl费米子，为我们研究Weyl费米子的物性提供了新的研究平台。

关键词：Y_2C 电子晶体、顺磁、Weyl费米子、第一性原理计算

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Liangliang Liu, Chongze Wang, et al. Theoretical prediction of Weyl fermions in the paramagnetic electride Y_2C Physicial Review B 2019, 99, 220401 Rapid Communications.

基金项目：国家自然科学基金（NO. 1177408）

M-P086

专题代号：M

哈密顿矩阵的基态普适关系及其应用

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摘要：矩阵的本征值问题是现代物理学中的首要问题之一。而量子多体系统由于其巨大的体系自由度导致对应的哈密顿矩阵无法直接对角化，从而对理论研究造成很大困难。在本工作中，我们首先通过数值方法对大量随机矩阵进行了研究，发现对于非对角元不大于零的实对称矩阵，基态本征矢和矩阵元之间存在普适的关联。对于对角元不占优的矩阵，基态本征矢中每个基矢的系数 g_i 与对应行矩阵元的和 S_i 之间近似呈线性关系 $g_i = -S_i$,且误差随矩阵维度的增大而迅速减小。对于对角元占优的矩阵，g_i 和 S_i 之间的标度关系虽然偏离线性，但仍保持整体上的单调关系，并且可以用幂函数来近似拟合。我们将这

种普遍规律称为基态标度关系。

作为上述基态标度关系的初步应用，我们研究了量子多体领域中的两个重要模型，即一维 Hubbard 模型以及一维和二维横场 Ising 模型。在研究它们的基态后，我们发现这些模型可以很好地由上述基态标度关系描述。进一步，通过比较基态能量我们发现，利用基态标度关系得到的结果与严格值非常接近，明显优于平均场的结果。这个关系提供了一种直接计算基态波函数而不需要进行对角化的新思路，其具有简单、受体系大小影响较小的优点。

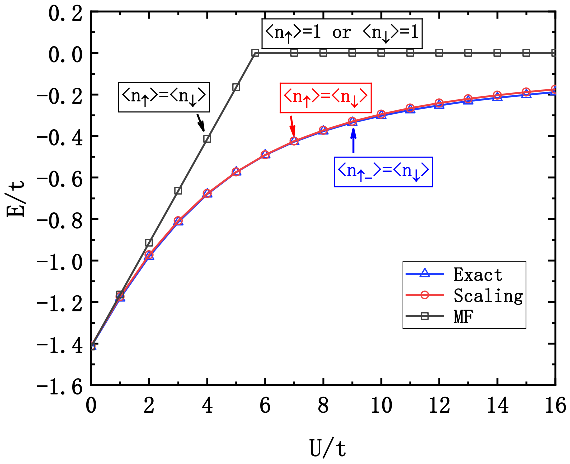

图 1　根据基态标度关系(Scaling)、平均场近似(MF)以及精确对角化方法(Exact)计算得到的 Hubbard 模型基态能量对比。

关键词：量子多体理论，哈密顿矩阵，基态，基态标度关系。

M-P087

专题代号：M

利用机器学习方法寻找 Heusler 合金中的高自旋极化铁磁材料

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摘要：目前，机器学习方法在材料科学上应用已十分广泛，这类方法可充分利用现有的广泛数据，加快材料研究进程。我们设计了一个在 Heusler 合金中搜索稳定的高自旋极化铁磁体材料的工作流，该工作流由多个深度神经网络(DNN)模型组合而成，其预测晶格常数模型的平均绝对误差（MAE）约为 0.10Å，形成能的 MAE 约为 92 meV/atom，预测自旋极化率模型的相关系数高于 0.91。在此工作流的帮助下，我们对 10557 种未知特性的 Heusler 合金的晶格常数，形成能和自旋极化率进行了预测，根据条件筛选后得到了 158 种可能具有热力学稳定的高自旋极化(HSP)的铁磁材料。其中，56 种合金在已有文献中被

报道为半金属材料（100%自旋极化率），80 种热力学稳定的 HSP 合金是未被报道过的，并有望在实验中制备。最终，我们发现了 5 种有自旋电子学应用前景的半金属铁磁材料，其中 Co_2CrB 有明显半金属性质，居里温度高于室温。在大数据背景下，结合机器学习方法可不受限于计算机算力，进行海量材料数据搜索与分析，这为新型材料的探索打开了新思路。

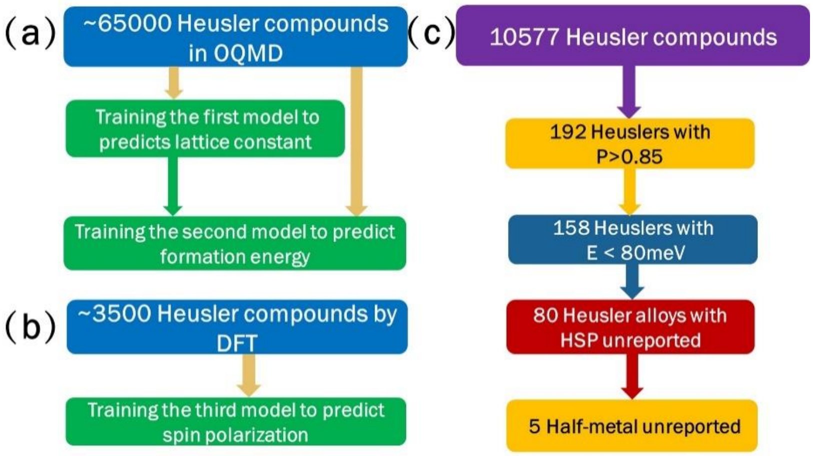

图 1 模型训练数据来源图(a)和(b)，材料搜索流程图(c).

关键词：机器学习，高自旋极化，铁磁半金属，Heusler alloys

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基金项目：国家自然科学基金项目（N0. 51572086, 51302085, 51402033, 11874273）

M-P088

专题代号：M

压缩和拉伸条件下 CeO_2 多晶型和相变的第一性原理计算

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摘要：本文基于密度泛函数理论（DFT），研究了 CeO_2 在萤石型（空间群 Fm-3m）、高钙石型(空间群 Pnma)、马氏体型(空间群 Pnnm)和金红石型(空间群 $P4_2/mnm$)的的结构、相变、电子、弹性和热力学性质。通过 PBE＋U 方法，获得了 CeO_2 多晶型物的基态性质，包括结构参数，电子结

构和力学性能，并与报道和实验结果值进行了比较。由萤石型向高钙石型结构转变的相变压力分别为 28.3GPa。电子性质对压力的依赖意味着在压缩和拉伸载荷下相变的带隙会缩小。通过对声子的计算，预测了 CeO_2 的所有相在该环境压力下是稳定的。给出了四种 CeO_2 晶型的热容、体积模量、吉布斯自由能和热膨胀系数随温度的函数关系，并通过 PBE+U 计算得到的 CeO_2 与实验结果数据吻合较好。

关键词：声子　相变　密度泛函数理论

基金项目：国家自然科学基金（NO. 11604029）

M-P089

专题代号：M

Unconventional Deformation Potential and Half-Metallicity in Zigzag Nanoribbons of 2D-Xenes and Group-IV Binary Compounds

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ABSTRACT：Realization of half-metallicity (HM) in low dimensional materials is a fundamental challenge for nano spintronics, which is a critical component for developing alternative generations of information technology. Using first-principles and SCC-DFTB calculations, we reveal unconventional deformation potential for zigzag 2D-Xenes and group-IV binary compounds nanoribbons (NRs). Both the conduction band minimum (CBM) and valence band maximum (VBM) of the edge states are of negative deformation potentials. This unique property, combined with the spin-polarization, and localization of the edge states, enable a strain way to induce spin-splitting and further the HM by inhomogeneous strain pattern, such as a simple in-plane bending. Indeed, our calculation using the generalized Bloch theorem reveals the predicted spin-splitting in bent zigzag 2D-Xenes and group-IV binary compounds NRs. As such, the HM can be achieved by hole or electron doping. Furthermore, the magnetic stability of the long range magnetic order for the spin-polarized edge states is maintained well against the bending deformation. These aspects indicate that it is promising to realize the HM in low dimensions with the zigzag 2D-Xenes and group-IV binary compounds NRs.

Key words：half-metallicity, zigzag Nanoribbons, unconventional deformation potential

基金项目：国家自然科学基金项目（No. 2017YFA0303400, No. 11674022 和 No. U1930402）

M-P090

专题代号：M

非平衡流和多相流的离散 Boltzmann 建模与模拟

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摘要：非平衡与多相复杂流动问题广泛存在于自然界和工程实践中，如超新星爆发、飞行器穿越稀薄大气层、微/纳尺度机电器件、页岩气开采、发动机中燃料的混合与燃烧等都会涉及。对于流动系统非平衡程度的表征一般是采用一个无量纲数，即 Knudsen 数（Kn），它定义为分子间平均自由程（λ）与系统特征尺度（L）之比，即 $\mathrm{Kn}=\lambda/L$。可以看出当流体分子间平均自由程较大、系统特征尺度较小、或者流体中存在界面和宏观量梯度时（相当于局域特征尺度小），系统的非平衡程度都会增强。

钱学森先生在研究稀薄气体动力学时最早提出，可以根据 Knudsen 数将流动区域划分为连续流、滑移流、过渡流和自由分子流。传统的流体力学基本方程（Navier-Stokes，NS）是基于连续性介质假设建立的，其本质上只适用于连续流情形；到了滑移流区，主流区的流动特征还可以近似用 NS 方程来描述，但需在边界附近考虑滑移修正；到了过渡流区，NS 方程中的线性本构模型，即牛顿粘性定律和傅立叶导热定律都不再适用了，这时需要考虑采用高阶的流动动力学方程如 Burnett 方程、Grad 矩方法、Eu 方法等。而研究表明，基于非平衡统计物理学的 Boltzmann 方程在以上整个流域内都是适用的，因此从这个层面上来说，Boltzmann 方程具有跨尺度的自适应性。

虽然 Botlzmann 有此优势，但是由于原始的 Boltzmann 方程中碰撞项含有高维积分，而且演化变量（分子速度分布函数）是一个六维空间的函数，求解过于复杂难以直接应用于实际问题的求解。近些年，北京应用物理与计算数学研究所许爱国研究员课题组基于离散 Boltzmann 方程，通过两步粗粒化建模，并在分布函数的动理学矩空间提取非平衡特征，发展出了适用于非平衡流动问题模拟研究的动理学模型——离散 Boltzmann 方法。目前该方法已成功应用于高速可压缩流动、燃烧与爆轰、流体界面不稳定性、多相流和非平衡相变等的研究中，获得了很多传统流体模型所不能提供的新认识。本报告首先介绍离散 Boltzmann 方法在非平衡流滑移区、过渡流区等的建模思路，包括动理学边界条件和高阶离散 Boltzmann 模型的构建；其次，基于该方法对速度滑移、温度跳变、Knudsen 曲线、非稳态壁面加热、流体界面不稳定性等问题进行模拟；最后介绍离散 Boltzmann 方法在多相流和非平衡相变问题中的应用，建立熵产生速率与非平衡特征量之间的关系式，并对相分离过程中的熵产生特性进行系统分析。

关键词：非平衡流、多相流、离散 Boltzmann 方法、界面不稳定性、熵产生

基金项目：国家自然科学基金项目（NO. 11772064），河南省高等学校重点科研项目（NO.20A460022），中国工程物理研究院创新发展基金创新项目（NO.CX2019033），爆炸科学与技术

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M-P091

专题代号：M

通过铁弹性控制二维 α-MPI (M = Zr, Hf)中各向异性电子行为的方向

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摘要：开发新颖器件迫切需要实现对二维材料电子行为的方向控制。目前，这方面的主要障碍之一是缺乏可行的控制手段。作为一种可行的方法，有两个关键因素必不可少：一个是“可切换的”，另一个是“精确的”。在此，我们提出二维铁弹材料相转变具有可切换性和精确性[1,2]，可以通过铁弹转变实现对各向异性电子行为的方向控制。通过第一性原理计算，我们发现 α-MPI (M = Zr，Hf) 单层不仅具有各向异性特征的超高载流子迁移率，而且还表现了出优异的铁弹性。[3] α-MPI 单层的铁弹转变势垒适中，铁弹性信号明显，有利于其在非易失性存储器件中的应用。同时，α-MPI 单层在 y 方向的载流子迁移率极高，而在 x 方向迁移率较低，说明载流子具有定向迁移的特征。这种共存表明，α-MPI 单层发生 90°铁弹转变后，具有空间各向异性的电子行为将发生可预知的变化：各向异性电子行为也将随铁弹转变旋转 90°。因此，采用铁弹转变可以实现对 α-MPI 单层中载流子迁移行为的方向控制。我们的研究结果为设计新颖可控电子器件提供了一种优异的方案。

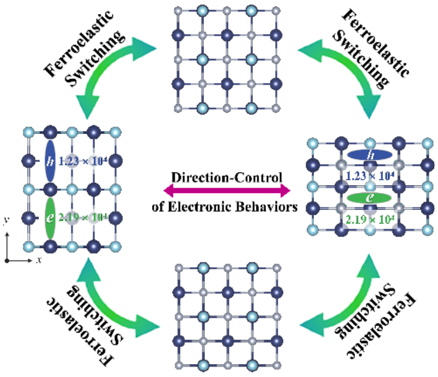

图 1 铁弹性控制 α-MPI (M = Zr，Hf)单层中各向异性电子行为的方向

关键词：二维材料 第一性原理计算 铁弹性 各向异性 载流子迁移率

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基金项目：国家自然科学基金（NO. 11804190）、山东省自然科学基金（NO. ZR2019QA011, ZR2019MEM013）、山东大学齐鲁青年学者项目、山东省泰山学者项目和山东省青年科技人才托举工程。

M-P092

专题代号：M

单层 Tl_2O 中非金属原子掺杂产生的谷极化

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摘要：除了电荷和自旋之外，电子还被赋予了额外的自由度，即谷自由度。谷自由度的利用，类比于电子学的电荷和自旋电子学的自旋，产生了被称为谷电子学的概念性电子应用。由于谷效应具有新颖的谷对比物理特性，因此具有很高的编码和处理信息的潜力。目前，许多二维材料已经被发现具有这种有趣的谷物理特性。例如，石墨烯、MoS_2、WTe_2等。制备谷电子学器件，关键的步骤是控制谷电子学器件的电子数，产生谷极化。虽然已经有了很多研究，但目前实现谷极化仍然具有挑战性。

利用第一原理计算，课题组团队提出可以通过非金属原子掺杂来实现单层 Tl_2O 中的特殊谷极化。单层 Tl_2O 是一种金属包覆半导体，由于其强大的自旋谷耦合，已被认为是一种有前途的二维谷材料。[1] 掺入 C 或 N 原子后，在单层 Tl_2O 中引入了磁行为。有趣的是，在考虑自旋轨道耦合的情况下，K 点和 K'点处的能量简并被打破，谷极化出现。特别指出的是，对于 N 掺杂的情况，缺陷态被隐没在价带中，因此，杂质态不会影响谷效应的性能，这是实际应用的理想选择。此外，两种情况下的谷极化都可以有效地利用磁场和外部应变来调控[2]，这些为实现谷极化和控制谷物理提供了一种实用的替代方法。

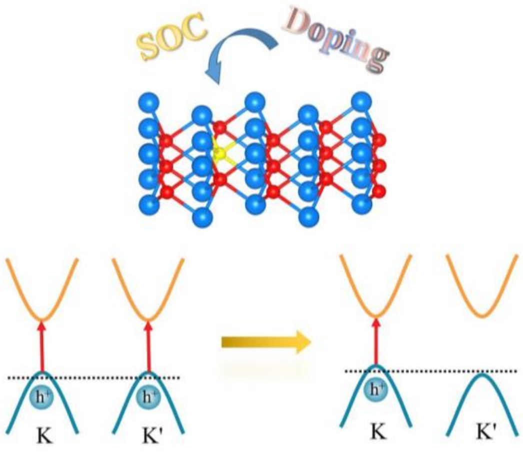

图 1 单层 Tl_2O 谷极化产生示意图

关键词：二维材料 谷极化

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M-P093

专题代号：M

单层 Ag_2S：二维双向拉胀材料

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摘要：泊松比是纵向结果应力与横向施加应力的比值的负数，是一个衡量材料力学性质的参数。根据弹性理论，三维各向同性材料的泊松比范围为 -1.0 ~ 0.5。因此，负泊松比材料（即拉胀材料）在理论上存在。拉胀材料在剪切模量、断裂韧性、热冲击强度、压痕阻力等方面具有优异的力学性能，在国防、工业、纺织、体育运动等领域有重要的应用价值。传统的拉胀材料往往是一些经过加工的三维材料。最近，二维拉胀材料受到人们的广泛关注。相比于传统拉胀材料，二维拉胀材料在纳米器件中具有很大优势。另外，二维拉胀材料的负泊松比都是本征的，不需要再另外加工。

课题组团队通过第一性原理计算研究了单层 Ag_2S 的电子性质和力学性质。研究表明，单层 Ag_2S 具有热力学、动力学与机械力学稳定性，是一个间接带隙半导体，具有各向异性的杨氏模量和负泊松比。此外，单层 Ag_2S 能够表现出拉伸膨胀现象。更为重要的是该材料的负泊松比不仅存在于面内方向，而且存在于其面外方向，这意味着该材料具有稀有的双向拉伸膨胀现象。这在之前关于拉胀材料的报道中是较为罕见的。

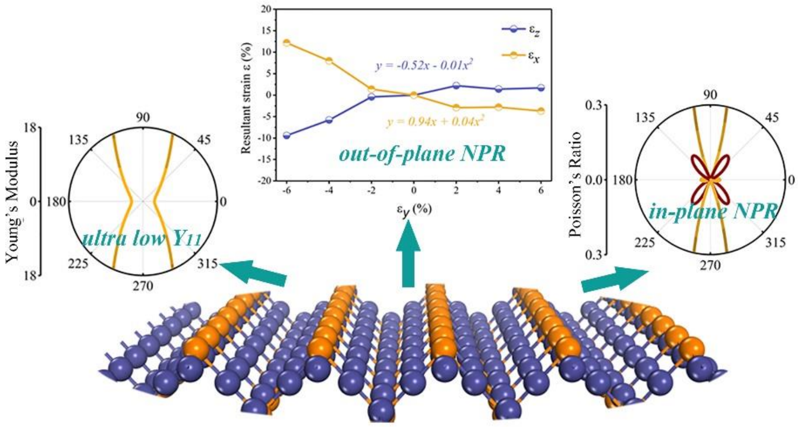

图 1 二维拉胀材料 Ag_2S

关键词：单层 Ag_2S　二维拉胀材料

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基金项目：国家自然科学基金项目（NO.11604213，11374190，21333006）等

M-P094

专题代号：M

仿生材料在氢能源中的应用

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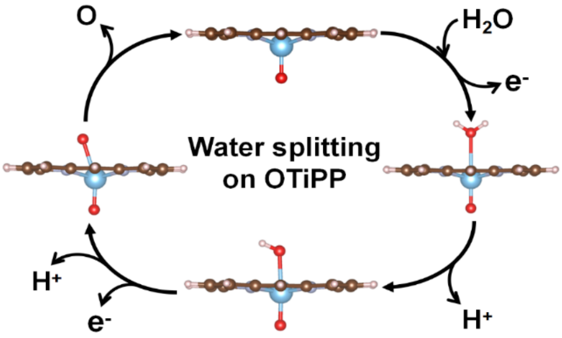
摘要：随着全球资源短缺和生态环境恶化，清洁能源和可再生能源的研究和开发具有重要意义。【1】利用第一原理计算寻求最佳的分解水的途径，我们首先研究了生物分子卟啉（MPP）（M=Mg、Ba、Sc、Ti、V、Cr、Mn、Fe、Co、Ni、Cu 和 Zn）催化水分解。在这些体系中，TiPP 体系在释放电子后是最有效的水分子分解催化剂，可高效分解水分子中的两个氢原子。TiPP 和剩下的氧原子形成了非常稳定的结构 OTiPP。卟啉分子释放电子需要外界输入能量，可使用太阳能来输入能量。H_2O+OTiPP 能以 6.76 eV 势垒释放电子。OTiPP 在释放电子后，能有效地催化水分子解离出两个自由的氢原子。值得注意的是，该解离过程是是一个放热过程，反应效率非常高。氧原子的解吸附过程，是一个具有 0.72 eV 势垒的吸热过程。H_2O+OTiPP 系统可以很容易地恢复到原来的状态 OTiPP。通过我们提出的势垒转移效应的作用下，OTiPP 可以成为水分解制氢的可持续循环催化剂。必须强调的是，为了释放电子以保持循环催化过程的可持续性，卟啉系统需要被注入能量，这种能量很容易从太阳能中获得。值得再次强调的是，在形成 OTiPP 系统,以及在 OTiPP 系统上分解水的整个过程中，只需要水和 TiPP，而不需要任何其他材料，最终产物只有 H_2 和 O_2。因此，这就确保了整个催化过程是非常干净的，没有任何污染，并且 OTiPP 体系可以恢复到原来的状态，这意味着它可以持续循环利用。这项研究将有助于设计有效的催化剂来分解水或其他氧化物分子，如二氧化碳和二氧化硫。由于整个催化过程可持续、没有任何污染，所以该方法

为未来清洁能源的发展和新型仿生光合成技术的发展开辟了新的途径。



$$2H^{+}+2e^{-}\rightarrow H_{2}$$

图 1 氧钛卟啉（OTiPP）可持续分解水分子制氢

关键词：仿生材料，清洁新能源，卟啉分子

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基金项目：国家自然科学基金项目（N0. 11474123）等

M-P095

专题代号：M

Cu-Zr 二十面体团簇(以 Cu 为心)化学序与其本征物性间的关联

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摘要：遗传性的局域五次对称性（LFFS）原子团及其联结存在于 Cu-Zr 非晶中是一个客观事实，它与 Cu-Zr 非晶的玻璃形成能力密切相关。本工作以液态 Cu-Zr 合金的快凝过程为背景，选取孤立 Cu_nZr_{13-n} 二十面体团簇作为研究对象，结合分子动力学与密度泛函理论，考虑并给出因 Cu 与 Zr 原子彼此局域环境不同而产生的所有团簇构型，系统的开展能态与电子结构的研究，用化学序参数将原子局域环境与电子结构关联起来。经研究发现：①在以 Cu 为心的 Cu-Zr 二十面体团簇的壳层位置，同种元素的原子倾向于聚集在一起，异种元素的原子倾向于分离排列。更为重要的是，我们在研究过程中对 Spaepen－Cargill 参数与 Warren－Cowley 参数的物理意义做了进一步推广；❷同类原子彼此聚集并成键可以增强团簇的化学稳定性、降低费米能级上的电子数，即 Spaepen－Cargill 参数与团簇的电子结构

之间存在较大程度的关联；❸对以 Cu 为心的低能稳态 Cu_nZr_{13-n} (n = 6,7,8, 9) 二十面体团簇的差分电子密度与 Mulliken 布居分析得知，Cu-Zr 二十面体中共价键与离子键共存，成键态与反键态共存，且团簇在形成时壳层 Zr 与中心 Cu 原子是电子的提供者，壳层 Cu 是电子的获得者。该电荷转移方向是金属玻璃中以 Cu 为心的 Cu-Zr 二十面体团簇普遍遵循的规律，不随团簇的化学序参数及化学组分的变化而变化。

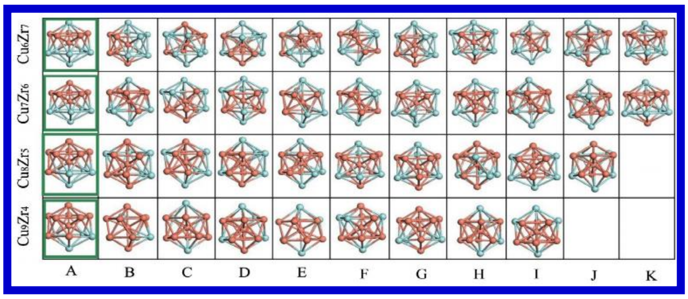

图 1 以 Cu 为心的 Cu-Zr 二十面体团簇示意图

关键词：金属玻璃，密度泛函，Cu-Zr 二十面体，电子结构，化学序

基金项目：江西省青年科学基金（批准号：20171BAB216001）、江西省教育厅科技项目（批准号：GJJ161242）、南昌师范学院博士启动基金（批准号：NSBSJJ2015034）和国家自然科学基金（批准号：51071065）资助的课题.

M-P096

专题代号：M

Trifunctional CoNx embedded graphene electrocatalysts for OER, HER and ORR

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The bifunctional catalysts for both oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) are of importance to the development of electrochemical energy systems such as reversible fuel cells, metal-air batteries, and water electrolyzers. Here, using the first-principles methods based on density functional theory (DFT), the Co and N codoped graphene systems (CoNx-gra, x = 1 - 4) with high ORR activity were further suggested as efficient OER catalysts. It was found that the activity on Co site of CoNx-gra towards ORR and OER would be affected by both the N-dopant concentration and configuration. The extrapolated overpotential of 0.37 V for either ORR or OER on CoNx-gra systems is comparable to those of noble metal benchmark catalysts. The origin of the activity stems from moderate hybridization between Co 3d orbital and p-orbital from O species, governed by the neighboring N coordination environment. Our results highlight the potential

application of transition metal and non-metal codoped graphene as efficient non-precious bifunctional catalysts.

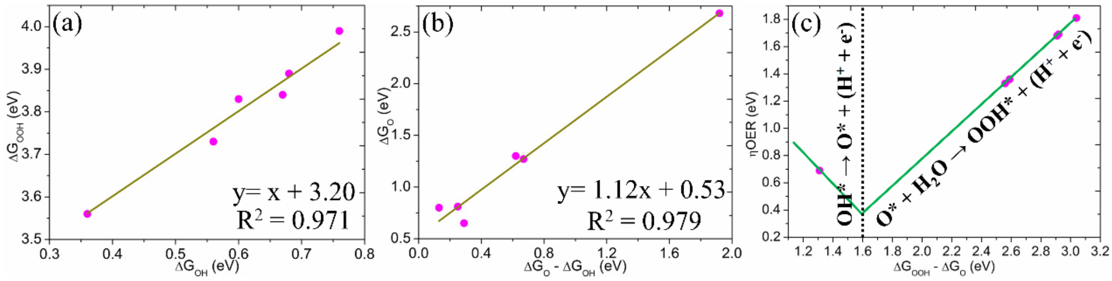

Fig. 1 The scaling relationship between △GOOH* and △GOH* (a), △GO* and (△GO* − △GOH*) (b), and the reverse volcano plot of ηOER vs (△GOOH* − △GO*) on CoNx-gra (c).

Keywords: Multifunctional, codoped graphene, doping concentration, ligands effect

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M-P097

专题代号：M

A first-principles study on the unrevealed electronic and optical properties of the LaAgOS-type copper oxychalcogenides

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Abstract: Transparent conducting oxides (TCOs) are well known for the outstanding performance in the field of optoelectronics. With large enough band gaps and p-type conductivity, LaAgOS-type oxychalcogenides have received extensive attention. Their exclusive properties, for instance, transparency, mobility, high dopability are intrinsically determined by the fundamental electronic properties. Herein, we studied the band structures, effective masses, and optical properties of a series of LaAgOS-type copper oxychalcogenides. The obtained

results show that the band gaps within HSE06 are expectedly in good agreement with the experimental data [1]. LaCuOCh (Ch = S, Se, Te) system possesses the band gap of 2.99 eV, 2.89 eV, and 1.77 eV, respectively. The band gap of LaAgOS (2.55 eV) is smaller than that of LaCuOS. Particularly, the band gap of LaCuSTe is predicted to be 0.48 eV, rather smaller than that of LaCuOTe (1.77 eV). It can be seen that atoms in the chemical elements of the same clan with larger atomic number decrease the band gaps of LaAgOS-type copper oxychalcogenides. A similar behavior was observed in the effective masses. LaCuSTe including S and Te atoms possesses the effective mass of 0.37 m_0 which is the slightest among LaAgOS-type systems. Thus we conclude that the atoms with larger atomic number prefer to the slighter effective masses, namely contributing the high mobility of the semiconductors. For p-type TCOs, holes transitions from the lower states to the unoccupied valence bands are called “second gap” [2]. In this study, we discussed the influences of this second gap on transparency of the LaAgOS-type copper oxychalcogenides. The calculated absorption coefficient (Figure 1) indicates that partial absorption appears in the visible range for LaAgOS, LaCuOS, LaCuOSe, and LaCuOTe. Among which, the LaCuOSe shows relatively good transparency. While the absorption coefficient of LaCuSTe is great even under visible light, which is corresponding to its small band gap (0.48 eV). Second gaps of LaAgOS-type copper oxychalcogenides follow the order: LaAgOS < LaCuOS < LaCuOSe < LaCuOTe <. LaCuSTe, which is roughly in accordance with the transparency of these materials. Namely, second gap may lead to degradation of the transparency for p-type semiconductors. It can be seen that LaCuOSe possesses the lower absorption coefficient in the visible range than the other copper oxychalcogenides, which combines with the predicted light effective masses, indicating the promising performances of the semiconductor LaCuOSe.

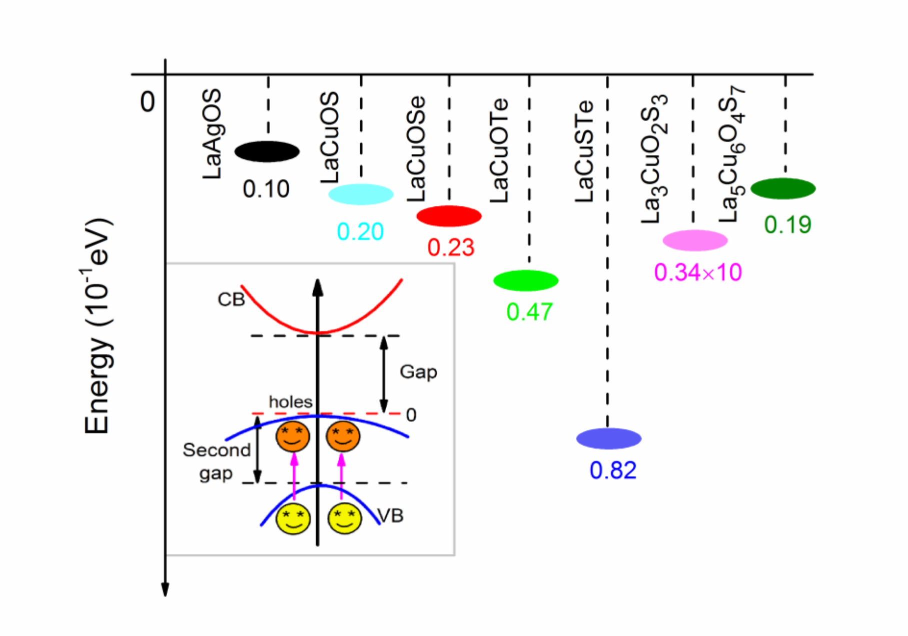

Figure 1 The second gaps of oxychalcogenides LaAgOS, LaCuOCh (Ch = S, Se, Te), LaCuSTe, La3CuO2S3 and La5Cu6O4S7.

Key words: TCOs; Effective mass; Second gap; Transparency; First-principles

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M-P098

专题代号：M

Grapheayne：拥有丰富光电及拓扑性质的低能碳同素异形体家族

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摘要：石墨烯是石墨的单原子层结构，由于其独特的二维构造，突出的物理、化学性质，以及它在微电子学、纳电子学，能源，化学、生物传感器的应用吸引了人们巨大的兴趣。石墨烯的零带隙阻碍了其在半导体器件集成中的直接应用。在打开石墨烯带隙的调控策略方面，人们已经做出了巨大的努力。当前有两种有趣的方法实现这一目的。一种是将石墨烯切割为纳米条带，其量子限制效应可以打开能隙，并且能隙的大小会随着可控的纳米条带的宽度震荡。另一种方法是在石墨烯 sp^{2}键中添加 sp 或 sp^{3}键，这可以通过化学功能化或者利用碳本身多样的成键特征实现。Graphyne 是一个突出的例子，它是由苯环（sp^{2}碳）和炔属连接（sp 碳）组成的一系列二维平坦的碳同素异形体。这个 sp-sp^{2}杂化键合特征可以显著的影响它的电子性质以及有助于调控它的带隙。例如，实验上合成的 graphyne 家族成员石墨炔是一个带隙为 0.5 eV 的半导体。

在这个工作中，我们基于以上两种方法在碳材料中对于能隙工程提出了一种新的策略。这个方案是通过乙炔连接（$-\mathrm{C}\equiv\mathrm{C}-$）组装石墨烯纳米条带构建出一个的碳网络结构[1]。随着纳米带的宽度变化，从而产生了一系列新的三维碳同素异形体— grapheaynes。通过第一性原理计算，我们展示了 grapheayne 家族拥有极好的稳定性。他们在能量上比实验合成的石墨炔以及理论上预言的拥有炔属连接的碳同素异形体更加稳定，并且他们的热稳定性可达到 1000K。在这个设计原则下，纳米条带的几何构造以及 sp-sp^{2}-sp^{3}杂化键赋予了 grapheayne 家族拥有多样的电子能带特征。我们发现，如果石墨烯纳米条带的宽度满足$n = 3p + 2$（p 是整数）的条件，那么这个体系是拓扑节点线半金属；否则，它是半导体。有趣的是，一些半导体（宽度为 3，4，7 和 10）拥有 1.07-1.87 eV 之间可调控的直接带隙，它可以媲美硅（1.1 eV），并且十分接近太阳能电池吸收材料的最佳带隙值 1.34 eV。这暗示着 grapheaynes 对于光电应用有着巨大的潜能，并且我们计算证实了它们比其他碳同素异形体以及其大部分光电材料具有更高的光吸收系数。我们的工作不仅揭示出 grapheayne 家族独特的原子构造以及显著的电子性质，而且也为催化剂、能源存储、分子筛、太阳能电池以及电子器件提供了一个具有应用前景的碳材料宝库。

关键词：三维碳同素异形体　直接带隙半导体　拓扑半金属　第一性原理

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M-P099

专题代号：M

单层 γ-SbP 和 γ-SbAs 中的二维铁电性

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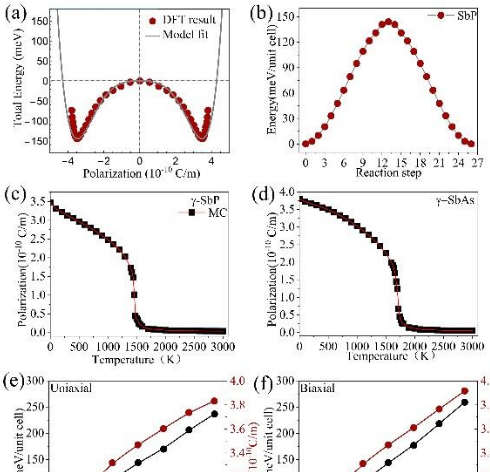
摘要: 近年来，铁电材料（FMs）因其在非易失性存储器件中的广阔应用前景而引起了人们极大的兴趣。先前铁电材料的研究主要集中在三维复合氧化物中（例如：$BiFeO_3$ 等）。然而，由于退极化场的影响，三维（3D）铁电材料在临界厚度以下会失去其铁电性，因此不能满足器件小型化的技术要求。为了克服这一缺点，人们致力于开发二维（2D）铁电材料。然而，截止目前，被提出的铁电材料少之又少。最近，SnTe，In_2Se_3 等 2D 铁电材料在实验上被成功证实激起了人们对 2D 铁电材料的进一步探索。利用第一性原理计算和蒙特卡罗模拟，我们确定单层 γ-SbAs 和 γ-SbP 是实现 2D 铁电性的优秀候选者。我们发现这两个系统都具有动力学和热力学稳定性。此外，它们具有非常大的电极化（单层 γ-SbAs 为 $3.80\times10^{-10}Cm^{-1}$，单层 γ-SbP 为 $3.47\times10^{-10}Cm^{-1}$）。而且，模特卡路的模拟结果显示单层 γ-SbAs 和 γ-SbP 的居里温度分别高达 1700 和 1400K，明显高于大多数早先报道的 2D 铁电材料。最后，我们还证明，在适当的应变下，两个系统的自发极化（P_s）和过渡势垒（E_b）可以进一步增加。这些有趣特性使单层 γ-SbAs 和 γ-SbP 有望用于非易失性存储器件和纳米级电子器件的未来应用。



关键词：二维材料，γ-SbX，铁电性，高居里温度

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基金项目：国家自然科学基金项目（NO. 11804190），山东省自然科学基金(NO. ZR2019QA011/ ZR2019MEM013)

M-P100

专题代号：M

Strain effect on magnetic transition and magnetic anisotropy energy in 2D two coordinated 5d transition metal

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Quantum information and spintronics devices, based on searching and manipulating magnetism, open up new questions in the studies of two dimensional materials. Using first-principle calculations, here we design a novel type of 2D metal organic frameworks (MOFs), which is composed of (1, 3, 5)-benzenetricarbonitrile (TCB) molecules linked with 5d transition metals (i.e., Hf, Ta, W, Re, Os, Ir), namely TCB-TM. Owing to their low coordinated, half-filled 5d electronic configuration, and suitable crystal field, robust ferromagnetism semiconductor with 63 meV bandgap, large magnetic anisotropy energy (19 meV/atom) and room temperature Curie temperatures (613 K) are found in TCB-Re monolayers. Remarkably, with the help of biaxial strain, a reversible magnetic transitions between ferromagnetic and antiferromagnetic have been found and the magnetic anisotropy energy is even increased up to 120 meV/atom. Meanwhile, large magnetic moment and room Curie temperature have been well preserved. To provide more insights into generally spin control mechanism, strain induced energy level regulating, bond reduction, orbital hybridization, magnetic interaction, and exchange coupling parameter have also been discussed. Our theoretical results point out that strain engineering is an effective method to manipulating spin and enhance the magnetic anisotropy energy to TCB-TM monolayer, which pave the way for experimental design of spin and magnetic storage devices.

Keywords: 5d transition metal; magnetic transition; magnetic anisotropy; strain

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M-P101

专题代号：M

层状外延多铁性复合薄膜电磁性能的数值模拟

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摘要：多铁性薄膜由于同时具有铁电有序和磁性有序并且在这两种有序态之间存在耦合效应，单相多铁性材料难以在室温下实现强的磁电耦合效应从而限制其实际应用。通过将具有强压电效应的铁电相与强磁致伸缩效应的铁磁相复合而成的多铁性材料理论上可获得室温下强的磁电耦合效应。但是，复合多铁性材料的磁电耦合效应与组成复合材料自身的性能、磁电相的体积比、测试条件(电磁场大小、频率、边界条件等)等因素相关。本文采用有限单元方法，对层状外延多铁性复合薄膜(2-2 型)，结合热力学理论和弹性理论，分析了外加磁场强度、边界条件、铁电相含量比和铁电薄膜面内应变对复合薄膜磁电耦合系数的影响。首先运用 Comsol 有限元软件中 PDE 模块对磁电多铁性复合材料进行分析计算，将磁电多铁性复合材料的力—电—磁耦合线性本构方程导入其 PDE 模块，对磁电多铁性复合材料 PZT(FE)/CFO(FM)薄膜进行计算分析。研究表明，边界条件的改变、铁电层所占比例的增大及杨氏模量的增加和面内应变的增加均能提高磁电多铁性复合材料的磁电耦合系数。本文通过蒙特卡洛方法，利用自旋翻转算法模拟 $BiFeO_3$ 铁磁薄膜的动态磁滞行为。研究外加磁场频率和振幅变化时铁磁迟滞特性的厚度依赖性。结果表明，随着薄膜厚度的增加，薄膜中的强铁磁耦合使计算出的磁滞特性发生了显著变化。

关键词：多铁薄膜 电磁耦合 有限单元法 蒙特卡洛模拟

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基金项目：国家重点研发计划（NO.2018YFB0703500）

M-P102

专题代号：M

基于第一性原理计算的银过饱和掺杂晶体硅的原子结构与光学性质

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摘要：深能级杂质超饱和掺杂晶体硅可以拓展光波吸收到近红外波段，符合 Luque 和 MartÍ 提出的中间带（IB）材料，低于带隙能量的电子跃迁到中间带并借助中间带跃迁到导带，大大地提升了吸收效率，中间带材料理论光电转换效率达到 63.2%，克服了 Shockley-Queisser 限制（极限效率为 31%）。

课题组通过第一性原理研究 Ag 超饱和掺杂晶体硅，以 Si_8 为单位在 2×2×2, 2×2×3, 2×3×3, 3×3×3 不同的超胞内构建可能出现的单原子结构（均匀掺杂）—替换结构(Ag_{Sub})，六边形结构(Ag_{HI})，四面体结构(Ag_{TI})，桥位结构(Ag_{BC})，能带结构或者 DOS 表明 Ag_{Sub} 能在费米能级形成中间带。建立银的双原子掺杂模型模拟非均匀掺杂，随着双原子距离增大，其形成能越大，体系越趋于均匀掺杂，而光学吸收扩展到近红外并吸收强度增强。为了进一步确定间隙结构是否对光吸收有贡献，我们构建了银替换结构与间隙结构（Ag_{HI}，Ag_{TI}，Ag_{BC}）的混合构型，与单原子银替换结构光吸收谱相比发现间隙结构有助于提高光吸收强度。

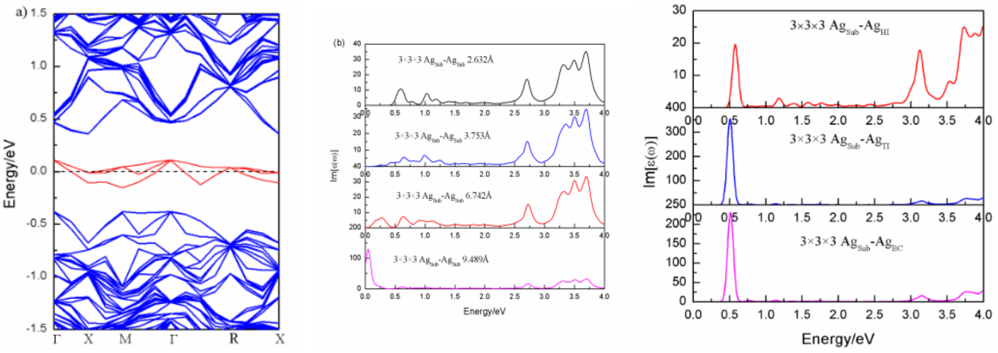

图 1. (a) 3×3×3 超胞替换结构能带图；(b) 不同距离点的双原子替换结构光吸收谱；(c)替换结构与间隙结构混合构型

关键词：中间带，超饱和掺杂，过渡金属 Ag， 电子结构，光学性质

基金项目：国家自然科学基金（NO. 11804083)

M-P103

专题代号：M

ZnO 基四元合金的电子结构和热力学性质理论研究

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摘要：ZnO 及其它 II-VI 族半导体材料由于其优异的性能而在光电、压电、热电、铁电等诸多领域被广泛应用。II-VI 等价离子掺杂的四元 ZnO 合金半导体对于开发波长可调的光电器件具有非常重要的意义，而对于掺杂过程中所出现的晶格畸变、掺杂元素含量限制、禁带宽度非线性变化、热力学稳定性等问题仍需亟待解决和进一步研究。本文采用基于密度泛函理论（DFT）的第一性原理计算，系统地研究了等价阴阳离子共掺的 ZnO 四元合金 $Be_xZn_{1-x}O_{1-y}S_y$[1]、$Mg_xZn_{1-x}O_{1-y}S_y$[2]、$Cd_xZn_{1-x}O_{1-y}S_y$和 BeMgZnO 等电子结构与相图。结果表明表明，MgZnOS 在低 Mg 和低 S 以及高 Mg 和高 S 含量下为六角纤锌矿结构；而在 Fig. 1(a)粉色区域中为闪锌矿结构；在高 Mg 和低 S 区域以及纤锌矿的富 MgS 端会出现岩盐矿相的 MgZnOS。在 S 含量为 0.05，Mg 含量为 0.75 时为三相的相平衡点。该结果对于实验上合成 MgZnOS 半导体材料和控制其相变机理过程具有很大的参考价值和理论指导意义。同时，由于多组元共掺引入更多的混合熵，使得在 ZnO 四元合金体系中溶解度间隙更小，更易形成合金相，能有效降低制备条件。此外，利用 HSE 杂化泛函和 Δsol 方法计算了 BeMgZnO 的带隙分布，如 Fig. 1(b)所示。通过多项式拟合分析发现，Be、Mg、Zn 在该四元合金体系中对带隙的影响具有高阶非线性相互作用，同时对于等价阳离子掺杂的 ZnO 而言，等价阴阳离子共掺的 ZnO 能够实现其在更大程度范围内的带隙调控，还能调节 ZnO 的价带和导带结构，改善其电子和空穴特性。

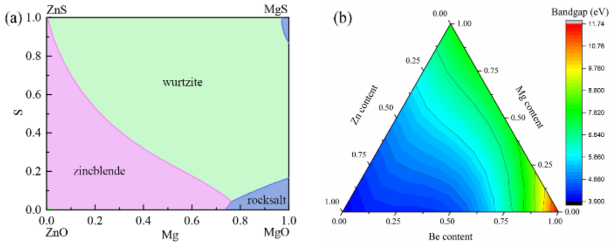

图1 (a) MgZnOS四元合金相图；(b) rocksalt相BeMgZnO四元合金带隙与元素含量的关系。

关键词： ZnO 基四元合金 第一性原理计算 相图

基金项目：国家自然科学基金项目（N0. 51572073，11574074，11774082，61874040）等

M-P104

专题代号：Ｍ

Effect of C2N-h2D Electrodes on the Rectifying Effects of Diblock Co-Oligomer Molecule Devices

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Based on nonequilibrium Green's function method in combination with density functional theory, we study the electronic transport properties of dipyrimidinyl-diphenyl molecules embedded in a carbon atomic chain sandwiched between zigzag graphene nanoribbon and different edge geometries C2N-h2D electrodes. Compared with the graphene electrodes, the C2N-h2D electrode can cause rectifying and negative differential resistance effects. For C2N-h2D with zigzag edges, a more remarkable negative differential resistance phenomenon appears, whereas armchair-edged C2N-h2D can give rise to much better rectifying behavior. These results suggest that this system can be potentially useful for designs of logic and memory devices.

Key words: Rectifying Effects ; Nonequilibrium Green's function; Electronic transport.

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M-P105

专题代号：M

Designing Perpendicular Two-dimensional Ferromagnetism in van der Waals Magnet $CrCl_3$ Monolayer

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Abstract: Among the recently widely studied van der Waals layered magnets CrX_3 (X=Cl, Br, I), $CrCl_3$ monolayer (ML) is particularly puzzling as it is solely shown by experiments to have an in-plane magnetic easy axis and, furthermore, all of previous first-principles calculation results contradict this. Through systematical first-principles calculations, we unveil that its in-plane shape anisotropy that dominates over its weak perpendicular magnetocrystalline anisotropy is responsible for the in-plane magnetic easy axis of $CrCl_3$ ML. To tune the in-plane ferromagnetism of $CrCl_3$ ML into the desirable perpendicular one, we propose substituting Cr with isovalent tungsten (W). We find that $CrWCl_6$ has a strong perpendicular magnetic anisotropy and a high Curie temperature up to 76 K. Our work not only gives insight into understanding the two-dimensional ferromagnetism of van der Waals MLs but also sheds new light on engineering their performances for nano devices.

KEYWORDS: *$CrCl_3$ monolayer, two-dimensional magnetism, van der Waals Magnet, perpendicular ferromagnetism*

M-P106

专题代号：M

The interplay of electronic, magnetic and structural properties of GdB_6 from first principles

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ABSTRACT: Gadolinium hexaboride (GdB_6) is a well known field emitter material that has been investigated for more than three decades. We perform a systematical density-functional theory (DFT) study of GdB_6 by using the generalized-gradient approximation and considering the electron interaction parameter *U*. The basic structural and electronic properties are carefully revised, as well as a strong *U*-value dependence in determining the antiferromagnetic (AFM) magnetic structures of Gd 4*f* electronic states. We found a small *U* (0~3eV) showing the most consistent experimental ground-state properties, which gives rise to a magnetic structure with a ground state of C-AFM and a second stable E-AFM. Moreover, we find the distortion modes of boron octahedron play an important role in the interaction between spin and lattice structures in this system. These results will deepen our understanding of the boron-based correlated rare earth compounds

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Key Word: Gadolinium hexaboride; density-functional theory; antiferromagnetic (AFM) magnetic structures; spin and lattice interaction

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M-P107

专题代号：M

磷酸胆碱在电场作用下的二维红外光谱图研究

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摘要：二维红外光谱已经被广泛应用于研究热平衡下分子的振动耦合和结构异构化现象，并且取得了很大的成就。磷酸胆碱分子是生物膜结构的基本组成单位，它的活性影响着多种疾病，比如心血管疾病。在人体中，神经信号的传导依赖于电势差，这种电势差在细胞膜间形成非常大的电场强度，数量级为 10^9 v/m，所以我们采用计算模拟的方法研究磷酸胆碱分子在 $-1.5\times10^9 \sim 1\times10^9$ V/m 电场范围内的二维红外光谱图，电场方向沿着 N-P 方向。研究结果表明电场影响磷酸胆碱分子与周围氨基酸形成氢键的数量，进而影响 P-O 键的振动耦合。还有电场并不显著影响磷酸胆碱分子的电荷密度分布，但是影响磷酸基团的极化方向。更重要的是当电场强度大小为 -1×10^9 V/m 的时候，磷酸胆碱分子就不再能进行旋转异构化了，这表明电场会影响细胞膜与周围蛋白的相互作用。而且我们得出结论电场会影响磷酸胆碱分子振动的非谐性和非谐频率。

关键词：磷酸胆碱、电场、、二维红外光谱、振动耦合、旋转异构化

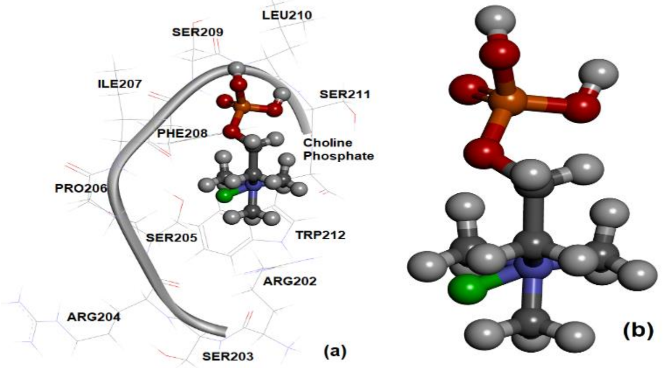

图 1，磷酸胆碱分子及其附近氨基酸示意图

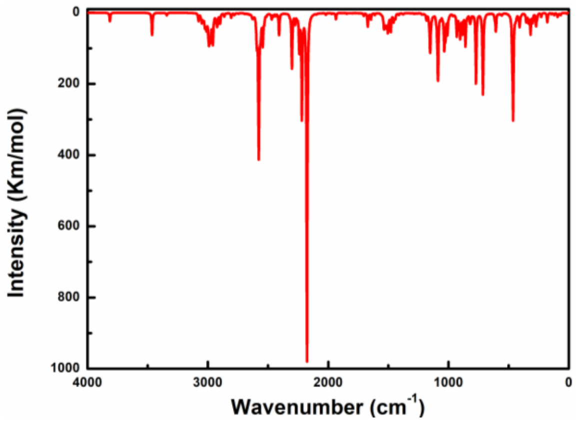

图 2，磷酸胆碱分子的模拟红外光谱图

【1】H. C. Ren, et al, Two-Dimensional Infrared Spectra of Cationic Dopamine under Different Electric Fields: Theoretical Studies from the Density Function Theory Anharmonic Potential, *J. Phys. Chem. C. 2018, 31, 17994-180004.*

基金项目：国防科技创新项目（17-163-12-ZT-0001-116-01, SWH2016LHJC-01）等

M-P108

专题代号：M

Vertical ferroelectric switching by in-plane sliding of two-dimensional bilayerWTe2

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ABSTRACT: The ferroelectric properties of the bilayer 1T’-WTe2 have been studied by the first-principles calculations. we have discovered that the polarization stems from uncompensated out-of-plane interlayer charge transfer, which can be switched upon interlayer sliding of an in-plane translation. The ferroelectric polarization directions further control the spin texture of bilayer WTe2, which may have important application in spintronics. Therefore, we propose a spin field effect transistor
(spin-FET) design that may effectively improve the spin-polarized injection rate. In addition, the lattice strain has been found to have an important influence on the ferroelectric properties of the bilayer WTe2.

Keywords: two-dimensional, WTe2, vertical ferroelectric, interlayer sliding, phase transition

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M-P109

专题代号：M

基于磁通环数据重建等离子体电流分布的研究

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摘要：等离子体电流的精确测量是托卡马克实验最关心的问题之一。其分布对于研究等离子体行为，了解装置的物理特征至关重要。本文介绍一种基于磁通环测量数据来重建等离子体电流分布的方法。与传统基于力平衡的平衡重建方法如 EFIT 相比，该类方法可以考虑并处理最外层闭合磁面以外的等离子体电流以及真空室腔壁涡流，并已经在小型球形托卡马克装置上成功测试【1】。

通过利用实验中磁通环的测量信息，考虑对磁通测量最重要的三项贡献：等离子体电流、极向场线圈电流及真空室腔壁感应涡流，建立了以下计算模型：1）首先，求解电路方程组，计算真空室腔壁感应涡流，求得真空室腔壁感应涡流及极向场线圈电流对磁通测量值的贡献，进而求得等离子体电流对各个磁通环的磁通贡献ψ_k^P（其中，上标 P 代表等离子体电流，下标 k 代表磁通环编号，ψ_k^P 即为等离子体电流磁通贡献测量值）；2）建立等离子体电流分布模型，将等离子体电流拆分成四个半椭圆，这四个半椭圆的分布函数共含有 7 个参量。从而可以通过电流丝累加模型【2】计算出等离子体电流在各磁通环产生的磁通量ψ_k（即为等离子体电流磁通贡献计算值）；3）基于最小二乘法，采用 MATLAB 中的 fminunc 最优化函数，最小化磁通的计算值ψ_k和测量值ψ_k^P之差，获得最佳等离子体电流分布参数。文献【1】中的原有方法在应用于中等规模的球形托卡马克装置时，出现最小二乘求解的计算量及存储量过大的问题。本文通过预设的等离子体电流和极向场线圈电流模拟发现，采用改进后的方法，等离子体电流值重建偏差基本在 0.05%以下，最小二乘残差基本处在 10^{-5} 量级，单个形状分布的重建时间约为 10s。

下一步将结合实验数据进行更详细的对比分析，并与传统方法相互校验。

关键词：等离子体 磁通环 电流重建 最小二乘 球形托卡马克

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M-P110

专题代号：M

用“约化 R-矩阵”模型研究质子-质子散射积分截面

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孙业英　　　　　　　　（清华大学 材料系）
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(2019-08-23)

用“约化 R-矩阵”理论程序 RAC，同时地和系统地分析了 0.35-56 MeV 能区全部的质子-质子散射微分截面实验数据，获得了很精密的拟合。由此获得了该能区的扣除库仑长程效应的质子-质子核散射微分截面和相应的积分截面。 将 RAC 积分截面与用参数化公式计算得到 pp 积分截面相比，在大于 20MeV 区域两者比较接近，但在 5-20MeV 区域，二者差别最大值约 10%。在 0.35-0.66MeV 区域，RAC 的计算值与用特洛伊木马方法给出的结果比较接近。此外，RAC 的 PP 积分截面值与美国阿拉莫斯国家实验室给出的中子-中子散射积分截面值很接近。本工作的创新性在于，以往只能用近似的经验公式估计较高能区的质子-质子核散射积分截面，而且得不到 0-180 度的微分截面，这里用“约化 R-矩阵”理论程序 RAC，可以给出准确的 0.35-56 MeV 能区的 pp 积分截面和微分截面。这个数据对优化输运理论计算具有重要的科学价值。

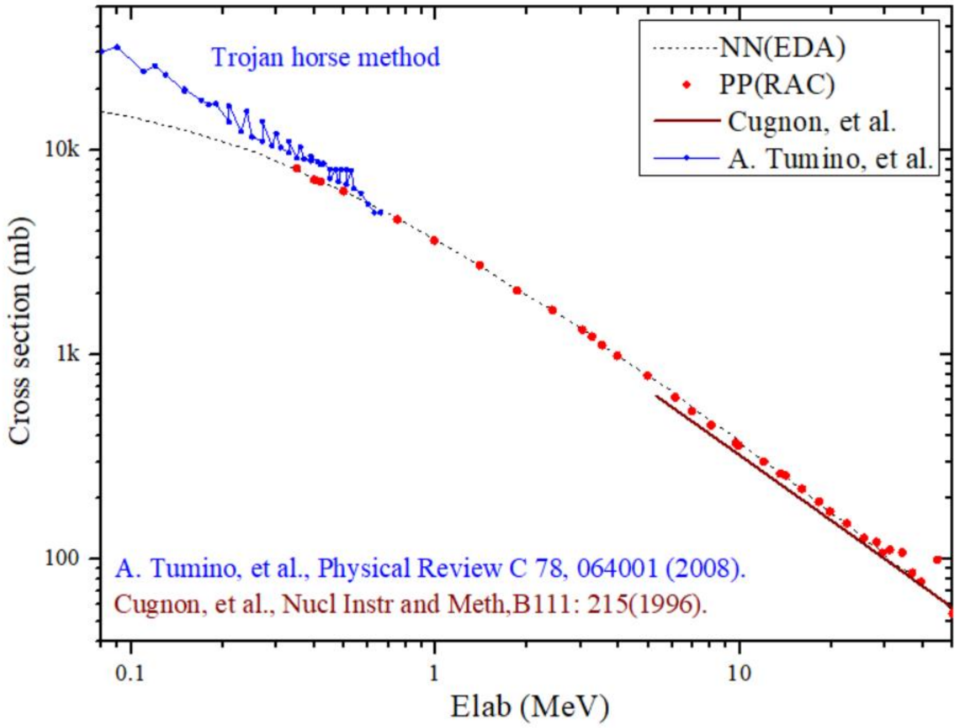

图 1：质子-质子散射积分截面。其中，红点为 RAC 给出的计算结果；蓝点为特洛伊木马方法计结果；暗红实线是参数化公式计算结果；黑虚线是阿拉莫斯国家实验室给的中子-中子散射积分截面。

M-P111

专题代号：M

Effect of Structural Disordering on Magnetic and Magneto-optical Properties of Fe_3Si

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The electronic, magnetic, transport and magneto-optical properties of the $D0_3$ and amorphous Fe_3Si are investigated by using the first-principles calculations. Pair correlation function analyses for the amorphous Fe_3Si obtained by initio molecular dynamics (AIMD) simulations showed that Si atoms prefer to bond with Fe atoms in the amorphous structure. The increase of Si neighbors purges the magnetization of Fe, while a small number of Si neighbors is beneficial for the enhancement of spin polarization at the Fermi level because of Si→Fe charge transfer. The structural disordering significantly alters magneto-optical Kerr effect, but not as strong on the anomalous Hall effect. The intrinsic anomalous Hall conductivity (AHC) of $D0_3$-Fe_3Si is 237 $(\Omega\ \mathrm{cm})^{-1}$ at room temperature and can be tuned to a high value of 1127 $(\Omega\ \mathrm{cm})^{-1}$ when the Fermi energy is lowered by -0.28 eV. In contrast, the AHC of amorphous Fe_3Si varies slowly with the shift of the Fermi level, indicating that it is insensitive to doping or gating. The Kerr rotation angle shows two main peaks in the energy range of 0~4 eV for the $D0_3$-Fe_3Si, whereas the first peak disappears when the structure becomes disordered. Our studies provide comprehensive data for FeSi alloys around this concentration ratio and the overall physical insights should be useful for the design of amorphous spintronic materials.

Key words: Fe_3Si, Anomalous, Hall effect, Kerr rotation, First principles calculation

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M-P112

专题代号：M

基于范德华铁磁半导体异质结构的可逆逻辑磁光控制设计

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摘要：铁磁半导体是实现自旋电子学同时利用电子电荷和自旋目标的最有前途的物质家族。基于层状铁磁半导体材料的新型自旋电子器件的出现为二维磁、磁电和磁光材料的概念设计提供了诱人的机会。由于异质结构无与伦比的兼容性，由二维材料组成的磁性异质结构正在积极扩展。这里，我们提出双层范德华铁磁半导体异质结的光激发双带边跃迁模型，以实现磁场可逆调控的光电流信号的逻辑输出。基于第一性原理计算，以 $CrBr_3/CrCl_3$ 异质结为例验证这一模型，我们主要阐明两个基本问题。一个是实验中实现范德华层状异质结可以不受晶格失配的约束，而考虑到异质结受应力的变化，会使 $CrBr_3/CrCl_3$ 的 CBM 带边的相对位置会发生变化，因此我们给出了带边相对位置随应力变化的相图。另一个是验证了堆叠方式及层间磁相互作用对能带结构基本没有影响。最后，我们模拟了磁场可逆调控 $CrBr_3/CrCl_3$ 的磁滞回线，并提出其他可能的铁磁半导体异质结组合，扩展了实验和未来应用铁磁半导体异质结构的可用

的功能。

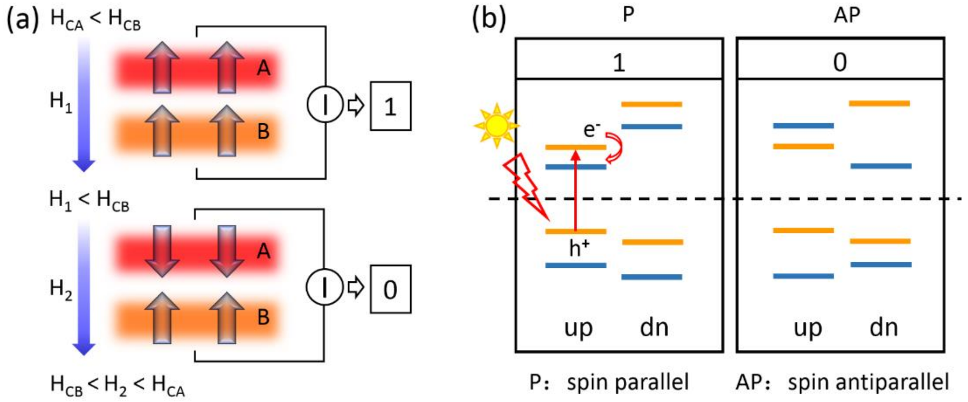

图 1 基于范德华铁磁半导体异质结构的光激发双带边跃迁模型机理图

关键词：二维材料，异质结，铁磁性，磁光控制，第一性原理

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M-P113

专题代号：M

二维本征高温铁磁半金属 Cr_3X_4 (X= S, Se, Te) 的第一性原理预测

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摘要：最近具有室温铁磁性和完全自旋极化的二维本征磁性材料作为纳米级自旋电子器件最有潜力的候选材料之一，受到了科研工作者的高度关注。然而，由于弱铁磁超交换相互作用以及二维铁磁材料中的自旋极化不完整使得目前已经实现的铁磁材料的居里温度（T_C）仍然远低于室温，这严重的限制了实际应用。基于第一性原理计算，我们报道了一系列 Cr_3X_4（X = S，Se，Te）单层，其中两种氧化态的 Cr 原子的共存导致了双交换相互作用发生，从而大大增强了铁磁耦合。 在自旋哈密顿量的精确解下， 他

们的 T_C 可以从磁化率和热容的峰位置准确地获得，其中 Cr_3Se_4 和 Cr_3Te_4 单层的 T_C 可分别高达 370 K 和 460 K。自旋极化计算进一步证明 Cr_3Se_4 和 Cr_3Te_4 单层是铁磁半金属，在理想情况下可以实现 100%自旋极化的电流。同时，我们确定了它们动力学和热力学稳定性，并提出了一种可能的合成策略。这项工作不仅为纳米级自旋电子应用提供了两种有竞争力的铁磁候选材料，而且还表明双交换相互作用可能是实现二维室温铁磁半金属的方案。

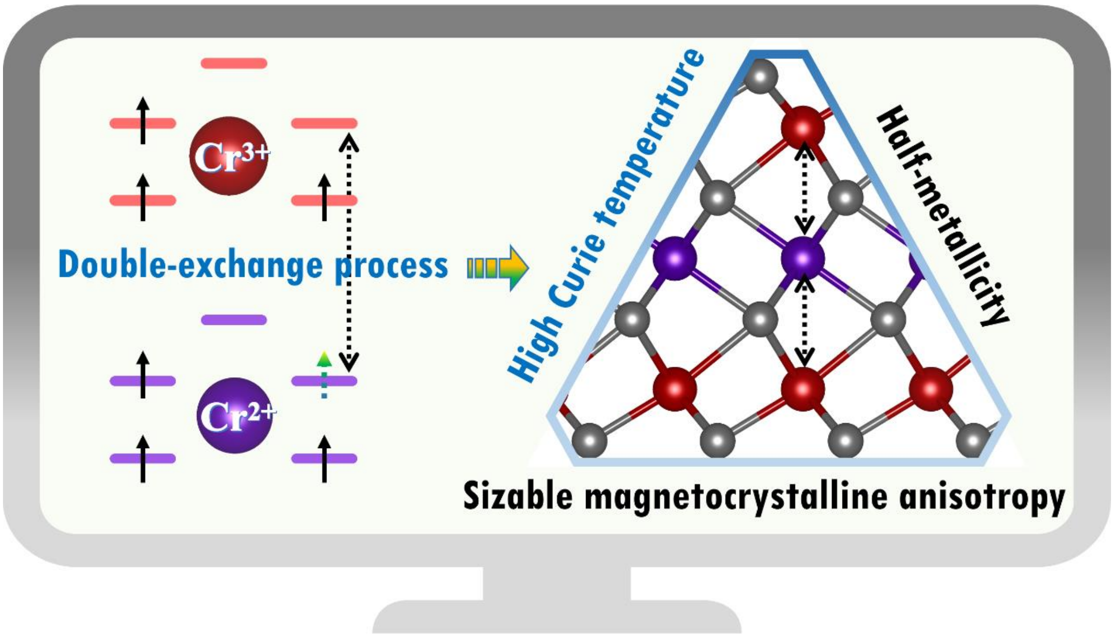

图 1 通过双交换过程使二维铁磁半金属获得高的居里温度。

关键词：二维，铁磁半金属，双交换，高居里温度，第一性原理

M-P114

专题代号：M

单层 C_4N_3H：一种二维有机狄拉克体系的结构设计及物性研究

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摘要：石墨烯和拓扑绝缘体研究的快速发展导致了一门名为“狄拉克物理”的新兴领域建立起来。这个领域研究的对象是一类具有狄拉克锥的特殊材料（即狄拉克材料）。狄拉克材料的重要特征是其能带在费米能级处具有线性的色散关系。这导致了材料中的载流子的行为类似于无质量狄拉克费米子，因此会出现很多新颖的物理现象，例如载流子的弹道传输，

克莱恩隧穿，各种量子霍尔效应，等。狄拉克材料的这些优势使得它们在高速、低能耗电子器件中具有广泛的应用前景。随着电子器件尺寸的不断减小，迫切需要发展更多的二维狄拉克材料。根据广义 von Neumann-Wigner 定理，二维狄拉克材料需要同时满足三个条件：1)特殊的对称性；2）适当的结构参数；3）合适的费米能级和能带折叠。这导致二维狄拉克材料非常稀少，而二维有机狄拉克材料更是少之又少。迄今为止，人们只发现了两种二维有机狄拉克材料，并且都具有非常低的费米速度。因此，设计具有高费米速度的二维有机狄拉克材料具有很大的实际意义。

该研究基于吡咯分子的骨架设计了一种二维有机材料，并根据它的化学组份将其命名为 C_4N_3H。这个有机单层材料具有新颖的几何结构，在这种结构中均匀地分布着埃级尺寸大小的孔洞。这种体系在自由状态下具有很好的动力学、热力学和机械稳定性。更重要的是，该研究发现这种材料是一个二维有机狄拉克材料，它具有各向异性的狄拉克锥和非常高的费米速度（1.1×10^6 m s^{-1}）。这个费米速度比以往报道的二维有机狄拉克材料的费米速度高一个数量级，和石墨烯相当。在这种体系的能带结构中，狄拉克点位于 Γ 和 K 点的连线上，狄拉克态主要来自于体系中碳原子和氮原子的 $2p_z$ 轨道交叠而形成的扩展的 π 电子共轭体系的贡献[1]。

此外，基于第一性原理计算，我们还进一步研究了这种材料的机械性质以及拉伸应变对它的电子性质的影响。我们的结果表明，相比其它很多二维材料，C_4N_3H 非常软，具有很小的刚度系数，并且能够承受更大的应变。另外，我们发现这种材料具有明显的各向异性的弹性性能，在某些方向具有非常大的泊松比（大于 0.5）。我们还发现这种材料的狄拉克态在外加应变下非常稳固，仍能保持较高的费米速度。并且在外加应变的情况下，体系狄拉克态的来源没有发生改变。小的刚度系数、大的泊松比、稳固的狄拉克态和高的费米速度使得这种新提出的 C_4N_3H 体系在高速柔性电子器件中具有潜在的应用价值[2]。

关键词：二维材料，有机狄拉克材料，狄拉克态，费米速度，应变调控
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Two-dimensional half-metallic ferromagnets: $FeCl_2$ and $MnSe_2$

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Abstract: Two-dimensional (2D) half metal materials have received more and more attentions due to their unique electronic properties, which make them perfect candidates for spintronic device. Herein, we systematically investigate two kinds of 2D half-metallic transition-metal dichalcogenides (TMDs): 1T-phase monolayer (ML) $MnSe_2$ and $FeCl_2$. Our first-principles calculations show that both 1T-ML-$MnSe_2$ and $FeCl_2$ favor ferromagnetic ground states and possess a respective 6.39 eV direct band gap and 1.29 eV indirect band gap for one of the spin channels. The other properties including structure stability, magnetocrystalline anisotropy energy (MAE), interlayer van der Waals (vdW) coupling, and Curie temperature (T_c) are also

studied. Finally, we found that $FeCl_2$ bilayer, $MnSe_2$ bilayer and their vertical heterostructure all favor an interlayer antiferromagnetic (AFM) coupling; however, only the vertical heterostructure preserves a half-metallic feature in ground state。

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