

表面物理国家重点实验室

STATE KEY LABORATORY FOR SURFACE PHYSICS

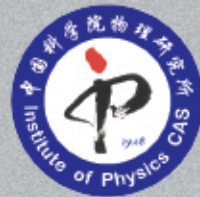
**2019-2020**

Annual Report 2019-2020

年报

中国科学院物理研究所  
INSTITUTE OF PHYSICS  
CHINESE ACADEMY OF SCIENCES

北京凝聚态物理国家研究中心  
BEIJING NATIONAL LABORATORY  
FOR CONDENSED MATTER PHYSICS



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## 实验室简介

表面物理国家重点实验室是由国家计委批准并资助建设的第一批国家重点实验室之一，于 1987 年建成并向国内外开放。首任实验室学术委员会主任为王迅院士，首任实验室主任为王鼎盛院士。林彰达，王恩哥，薛其坤，高世武曾先后担任实验室主任。现任实验室学术委员会主任为薛其坤院士，现任实验室主任为郭建东研究员。实验室拥有一支年轻的优秀科研团队，现有固定研究人员 31 名，在站博士后 10 名，在读研究生 103 名。实验室成立至今有 3 人（王鼎盛、薛其坤、王恩哥）被推选为中国科学院院士，11 人获得国家杰出青年科学基金支持，3 人获得优秀青年科学基金项目。

实验室以物质表面和界面为主要研究对象，使用高精度原子尺度实验工具，与理论方法密切结合，开展与信息科学、纳米科学和能源科学有直接联系的材料制备、物性表征、功能调控与物理机制等方面的研究。当前研究集中于发展原子级精度控制方法制备低维与纳米结构，发展多种自由度、高分辨率新型表征技术，以此为基础研究表面 / 界面各种新奇电子态、低维量子结构中的局域效应及其集体激发特性、以及相关的电子激发态超快动力学特征等。实验室设六个课题组，研究内容包括：

- 低维结构物性调控及其原位电子显微学研究
- 表面原子过程与薄膜生长
- 单分子及表面元激发的测控和动力学研究
- 氧化物人工低维结构的生长与性能调控
- 低维量子材料的分子束外延生长和电子态调控
- 表面激发动力学和能源应用

在鼓励原创性基础科研工作的同时，实验室面向国家重大研究任务和战略性技术储备需求，努力促进各课题组学术方向的凝聚和合作。实验室目前承担国家重点研发计划项目、国家自然科学基金项目、中国科学院战略性先导科技 B 类专项及国际合作项目，在表面物理相关学科的一些领域取得了重要进展，研究工作得到了国内外学界的一致认可。2019-2020 年间，实验室在极性拓扑结构的原位观测、氧化物物性调控、界面超导机理、摩尔超晶格拓扑态、电荷序超快动力学、高压泵浦 - 探测超快光谱、高质量材料数据库等方面取得了一系列优秀的研究成果，在 SCI 收录期刊中发表论文 160 篇，其中 Science 1 篇，Nature 3 篇，Nature 子刊 9 篇，Physics Review Letters 10 篇，PNAS 1 篇，Journal of American Chemical Society 1 篇，Nano Letters 5 篇，Advanced Materials 2 篇。2020 年，孟胜获得基金委国家杰出青年基金项目支持。

实验室加快推进共享仪器建设，形成了集理论计算、低维量子结构制备、高空间分辨率观测、多自由度谱学以及输运性质测量等研究手段全面、完善的“低维量子结构表征与操纵平台”，包含 30 台 / 套大型仪器，在实验室内部共享并对外开放。继 2012 年创办“Recent Progress in Oxide Interfaces”年度系列研讨会以



## 实验室概况

来，实验室每年坚持主办量子材料低维结构方面的国际研讨会，吸引了这一新兴领域的众多国际专家来交流最新的研究进展，并开展长期稳定的科研合作。实验室还一直坚持推动“表面科学论坛”和“物理半月谈”活动，有效促进了学术交流和文化建设。

表面实验室的发展离不开前辈专家、各界朋友的关心与支持。在此谨向大家表示衷心的感谢！我们将继承发扬实验室的优良传统，团结一致，面向世界科学前沿和国家战略需求，再接再厉，力争取得更大的进步！

# INTRODUCTION

The State Key Laboratory for Surface Physics was founded in 1987 as one of the first ten state key laboratories in China. Prof. Xun Wang and Prof. Dingsheng Wang served the first term of the Academic Steering Committee Chair and Lab Director, respectively. Subsequent lab directors include Prof. Zhangda Lin, Prof. Enge Wang, Prof. Qikun Xue, and Prof. Shiwu Gao. The current Academic Steering Committee Chair is Prof. Qikun Xue and the Lab Director is Prof. Jiandong Guo. The Laboratory owns a young talented research team, including 31 regular staff members, 10 post doctors and 103 graduate students. Since the founding of Lab in 1987, three lab members (Dingsheng Wang, Qikun Xue and Enge Wang) have been elected to the Academy of Chinese Academy of Sciences, eleven have received National Distinguished Young Scientists Awards, three have received National Excellent Young Scientists Awards.

Our mission is to explore the fundamental aspects of novel phenomena at surfaces and interfaces, with a combination of atom-resolved experimental tools and first-principles calculations. Our research goal aims at fabrication, characterization and functionalization of artificial materials that have potential applications in information, energy and nano science. Current research activities include the controlled growth of low-dimensional quantum structures with atomic precision, development of novel instruments with high resolution in multiple degrees of freedom, and investigation with such novel tools on the localized phenomena as well as their collective behaviors at surfaces and interfaces, effects of the microstructure on macroscopic properties, and dynamic behaviors in excited electronic states. There are currently six research groups in the Lab:

- Emergence of Low-dimensional Structures and Their Atomic Mechanism by In-situ TEM Method
- Atomic Processes on Surface and Film Growth
- Detection, Control, and Dynamics of Single Molecules and Elementary Excitations
- Growth of Artificial Low-dimensional Oxide Structures and the Functionality Control
- MBE Growth and Electronic Properties of Low-dimensional Materials
- Surface Excitation and Energy Conversion

The lab encourages original research explorations, while we are also making great efforts to organize teams for major national projects. The Lab has been very active in undertaking major national scientific projects, including the National Key Research and Development Programs of Chinese Ministry of Science and Technology, the key projects of National Natural Science Fund of China, as well as the Strategic Priority Research Program (B) of the Chinese Academy of Sciences. Significant research progresses have been made in the Lab and have attracted lots of attention worldwide. During the year 2019-2020, series of significant progresses have been achieved in studies of polar topological structures, complex oxides, interfacial superconductivity, moiré superlattice, charge density wave dynamics, high pressure pump-probe spectroscopy and high-quality materials database. More than 150 SCI papers were published, including 1 in Science, 3 in Nature, 9 in Nature subsidiaries, 10 in Physics Review Letters, 1 in PNAS, 1 in Journal of the American Chemical Society, 5 in Nano Letters and 2 in Advanced Materials. Sheng Meng was awarded the National Natural Science Fund for Distinguished Young Scholar in 2020.

We have made major progresses in establishing the shared network of instruments. A comprehensive instrument platform was established with 30 sets of equipment for material computation, fabrication of low-dimensional structures,



## 实验室概况

high-resolution characterization, spectroscopy with multiple degrees of freedom, and electric transport measurements, etc. Following the first international workshop on oxide interfaces in IOP in 2012, we organize the series of the workshop annually. Worldwide experts in this emerging field have been attracted to exchange their latest progress and to initiate solid collaborations with IOP. To promote the exchange of scientific ideas, we organize the Surface Science Colloquium and the Semimonthly Forum on Physics. All these efforts have laid a solid foundation for our sustainable developments in the future.

We sincerely appreciate the tremendous helps and supports from all colleagues and friends around the world. Thank you for your continuous interest in the lab. We strive to work with our staff, students and friends for a bright future.



## 行政机构和管理

Organization & Administration

实验室主任：郭建东 研究员

Director: Prof. Jiandong Guo

实验室副主任：孟 胜 研究员

Deputy Director: Prof. Sheng Meng

## 历届主任

Successive Directors

第一届主任：	王鼎盛 研究员（院士）	
	Prof. Dingsheng Wang	(1987 - 1991)
第二届主任：	林彰达 研究员	
	Prof. Zhangda Lin	(1991 - 1995)
第三届主任：	王恩哥 研究员（院士）	
	Prof. Enge Wang	(1995 - 2000)
第四届主任：	薛其坤 教授（院士）	
	Prof. Qikun Xue	(2000 - 2005)
第五届主任：	高世武 研究员	
	Prof. Shiwu Gao	(2005 - 2009)

## 实验室概况

### 学术委员会

#### Academic Steering Committee


主任 Chairman	
薛其坤 教授 (院士)	Prof. Qikun XUE, Southern University of Science and Technology
副主任 Deputy Chairman	
王恩哥 研究员 (院士)	Prof. Enge WANG, Institute of Physics, CAS
委员 Members	
万立骏 研究员 (院士)	Prof. Lijun WAN, Institute of Chemistry, CAS
王鼎盛 研究员 (院士)	Prof. Dingsheng WANG, Institute of Physics, CAS
王 琛 研究员	Prof. Chen WANG, National Center for Nanoscience and Technology
王 牧 教授	Prof. Mu WANG, Nanjing University
王 兵 教授	Prof. Bing WANG, University of Science and Technology of China
牛 谦 教授	Prof. Qian NIU, University of Texas At Austin
包信和 教授 (院士)	Prof. Xinhe BAO, University of Science and Technology of China
江 颖 教授	Prof. Ying JIANG, Peking University
朱 星 教授	Prof. Xing ZHU, Peking University
刘 峰 教授	Prof. Feng LIU, University of Utah
李树深 研究员 (院士)	Prof. Shushen LI, Chinese Academy of Sciences
杨学明 研究员 (院士)	Prof. Xueming YANG, Dalian Institute of Chemical Physics, CAS
张振宇 教授	Prof. Zhenyu ZHANG, University of Science and Technology of China
何丕模 教授	Prof. Pimu HE, Zhejiang University
张坚地 教授	Prof. Jiandi ZHANG, Louisiana State University
张绳百 教授	Prof. Shengbai ZHANG, Rensselaer Polytechnic Institute
周兴江 研究员	Prof. Xingjiang ZHOU, Institute of Physics, CAS
姜晓明 研究员	Prof. Xiaoming JIANG, Institute of High Energy Physics, CAS
封东来 教授	Prof. Donglai FENG, University of Science and Technology of China
高鸿钧 研究员 (院士)	Prof. Hongjun GAO, Institute of Physics, CAS
郭建东 研究员	Prof. Jiandong GUO, Institute of Physics, CAS
贾金锋 教授	Prof. Jinfeng JIA, Shanghai Jiao Tong University
裘晓辉 研究员	Prof. Xiaohui QIU, National Center for Nanoscience and Technology




## 实验室概况

### 杰出人才

#### Outstanding Researchers

 中国科学院院士  
Academician, CAS

王鼎盛      Dingsheng Wang  
王恩哥      Enge Wang  
薛其坤      Qikun Xue (现在机构: 南方科技大学)

 国家杰出青年基金获得者  
National Natural Science Fund for Distinguished Young Scholar

1995 王恩哥      Enge Wang  
1996 薛其坤      Qikun Xue      (现在机构: 南方科技大学)  
2003 贾金锋      Jinfeng Jia      (现在机构: 上海交通大学)  
2007 白雪冬      Xuedong Bai  
2008 夏 钊      Ke Xia      (现在机构: 北京师范大学)  
2008 高世武      Shiwu Gao      (现在机构: 北京计算科学中心)  
2010 马旭村      Xucun Ma      (现在机构: 清华大学)  
2012 郭建东      Jiandong Guo  
2013 何 珂      Ke He      (现在机构: 清华大学)  
2018 吴克辉      kehui Wu  
2020 孟 胜      Sheng Meng

 国家海外青年学者合作研究基金获得者  
Joint Research Fund for Overseas Chinese Young Scholars

1999 张振宇 / 王恩哥      Zhenyu Zhang/Enge Wang  
2001 施至刚 / 薛其坤      Zhigang Shi/Qikun Xue



## 优秀青年科学基金项目

National Natural Science Fund for Excellent Young Scholar

2012 孟 胜 Sheng Meng

2013 王文龙 Wenlong Wang 陈 岚 Lan Chen



## 其他人才计划入选者

1995 王恩哥 Enge Wang

1998 曹则贤 Zexian Cao

薛其坤 Qikun Xue (现在机构: 南方科技大学)

2000 贾金锋 Jinfeng Jia (现在机构: 上海交通大学)

2002 夏 钊 Ke Xia (现在机构: 北京师范大学)

2004 高世武 Shiwu Gao (现在机构: 北京计算科学中心)

吴克辉 Kehui Wu

2005 郭建东 Jiandong Guo

2009 陆兴华 Xinghua Lu

梁文杰 Wenjie Liang

孟 胜 Sheng Meng

2014 王炜华 Weihua Wang

2018 刘 淼 Miao Liu

鲁年鹏 Nianpeng Lu

冯宝杰 Baojie Feng

2020 章一奇 Yiqi Zhang

田学增 Xuezheng Tian

# 实验室概况

## 研究组和研究方向

### Research Groups & Directions

#### ☑ SF01 课题组

低维结构物性调控及其原位电子显微学研究

Emergence of Low-dimensional Structures and Their Atomic Mechanism by In-situ TEM Method

- 二维材料可控制备与结构相变动力学研究  
Controllable preparation and structural transition of two-dimensional materials
- 功能氧化物氧迁移与结构物性调控研究  
Oxygen migration and physical manipulation of functional oxides
- 原位电子显微学方法与实验技术研究  
In-situ TEM method and related instrument technique

组 长: 白雪冬

成 员: 王文龙 许 智 王立芬 田学增 李晓敏 王 理

博士后: 左勇刚 陈 潘 王建林 陈子韬

#### ☑ SF03 课题组

表面原子过程与薄膜生长

Atomic Processes on Surface and Film Growth

- 氧化物离子调控及物性研究  
The ionic modulation and properties of oxides
- 水溶液的玻璃化及冷结晶  
Mechanisms of vitrification and cold-crystallization of aqueous solutions

组 长: 曹则贤

成 员: 鲁年鹏 纪爱玲 王 强 张凌云

#### ☑ SF05 课题组

单分子及表面元激发的测控和动力学研究

Detection, Control, and Dynamics of Single Molecules and Elementary Excitations

- 表面单分子动力学  
Dynamics behavior of single molecules on surface
- 单自旋量子态测控  
Detection and control of single spin quantum state
- 固态纳米孔 DNA 测序  
Solid state nanopore for DNA sequencing
- 超导、强关联、拓扑等关联量子材料的超快光谱学, 超快动力学和非线性光谱学  
Ultrafast spectroscopy, ultrafast dynamics, and nonlinear optical spectroscopy of correlated materials, such as superconductors, strongly correlated systems and topological materials.

组 长: 陆兴华

成 员: 赵继民 单欣岩

博士后: 刘海江 赵新佳

## 实验室概况

### ☑ SF06 课题组

氧化物人工低维结构的生长与性能调控

Growth of Artificial Low-dimensional Oxide Structures and the Functionality Control

- 氧化物界面二维电子体系的多自由度有序态  
Ordering of multiple degrees of freedom in the two-dimensional electron systems at oxide interfaces
- 二维材料及其与氧化物界面体系中的新奇物理现象  
Novel phenomena in two-dimensional materials and the interfaces with oxides
- 有机分子表面自组装结构调控低维磁性  
Low-dimensional magnetism tuned by the surface self-assembly of organic molecules

组 长: 郭建东

成 员: 孙 牧 王炜华 杨 芳 朱学涛 孟 梦 刘笑然

### ☑ SF09 课题组

低维量子材料的分子束外延生长和电子态调控

MBE Growth and Electronic Properties of Low-dimensional Materials

- 二维材料的分子束外延制备与表征  
MBE growth and electronic properties of two-dimensional materials
- 拓扑量子材料的电子结构研究  
Electronic structures of topological quantum materials
- $\pi$  共轭二维有机聚合物晶体的表面合成与物性研究  
On-surface synthesis and characterization of  $\pi$ -conjugated 2D polymeric crystal

组 长: 吴克辉

成 员: 陈 岚 冯宝杰 章一奇 程 鹏

### ☑ SF10 课题组

表面激发动力学和能源应用

Surface Excitation and Energy Conversion

- 激发态量子动力学研究及其在新能源和纳米器件的应用  
Excited state quantum dynamics research and its application in energy conversion and nano devices
- 发展先进的非绝热全量子化动力学模拟软件  
Development of state-of-the-art nonadiabatic quantum dynamics simulation software
- 建设国际一流的计算材料数据库  
Construction of world-class computational materials database

组 长: 孟 胜

成 员: 王恩哥 刘 淼 张 萃

博士后: 关梦雪 杨 庆 徐纪玉

# M 实验室成员名单 Members of Laboratory



## 研究人员 27 名 / Researchers



王恩哥  
Enge Wang

研究员，中国科学院院士，第三世界科学院院士  
Professor, Member of Chinese Academy of Sciences

### 研究方向 / Research Area

轻元素纳米新材料探索及其物理性质，原子尺度上的表面生长动力学，受限系统中水的行为与特性  
Novel nanomaterials based on light elements; Growth dynamics at atomic scale on surfaces; Behaviors of water in confined systems



白雪冬  
Xuedong Bai

研究员，杰青  
Professor, NSFC Distinguished Young Scholar

### 研究方向 / Research Area

原位电子显微学，原子分辨结构表征与物性调控，低维材料与表界面物理，离子输运及相变  
In situ transmission electron microscopy; Atomic-scale characterization and manipulation of structural properties; Low-dimensional materials and surface/interface physics; Ion transport and phase transition



曹则贤  
Zexian Cao

研究员  
Professor

### 研究方向 / Research Area

薄膜生长技术、过程与机理，新材料探索，水科学，低温等离子体，凝聚态表面，微结构与量子力学  
Thin film growth, the atomic process and mechanism; Exploration of the new materials; Water science research; Low temperature plasma and the condensed matter surface; Micro-structures and quantum mechanics



陈岚  
Lan Chen

研究员，优青  
Professor, NSFC Outstanding Young Scholar

### 研究方向 / Research Area

二维材料及其异质结，拓扑量子材料，扫描隧道显微学，表面物理化学性质  
Two-dimensional materials and their heterojunctions; Topological quantum materials; Scanning tunneling microscopy; The Physical and chemical properties of surface



郭建东  
Jiandong Guo

研究员，杰青  
Professor, NSFC Distinguished Young Scholar

### 研究方向 / Research Area

低维量子结构的设计制备与新奇物理性质，表面电子谱学分析  
Design & preparation of low-dimensional quantum materials and their novel properties; Surface electronic spectroscopy



陆兴华  
Xinghua Lu

研究员  
Professor

### 研究方向 / Research Area

表面单分子动力学研究，超快时间分辨扫描隧道显微学，纳米孔 DNA 测序技术研究  
Dynamics of Single Molecules on Surface; Ultrafast Time-Resolved Scanning Tunneling Microscopy; Nanopore DNA Sequencing

## 实验室成员名单



孟胜  
Sheng Meng

研究员, 杰青  
Professor, NSFC Distinguished Young Scholar

### 研究方向 /Research Area

激发态量子动力学, 能量转化和存储微观机制, 太阳能电池, 表面与水相互作用等

Excited state quantum dynamics; Energy conversion; Solar cells; Water-surface interactions



孙牧  
Mu Sun

研究员  
Professor

### 研究方向 /Research Area

低维纳米结构的生长与物性研究  
Fabrication and physical properties investigation of low dimensional nanostructures



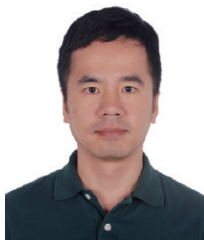
王文龙  
Wenlong Wang

研究员, 优青  
Professor, NSFC Outstanding Young Scholar

### 研究方向 /Research Area

轻元素低维材料的控制合成与电子结构调控, 电化学与光电催化过程中的表界面问题

Controlled synthesis and electronic structure control of light-element low-dimensional materials; Surface and interface problems related to electrochemical and/or photoelectrochemical processes



吴克辉  
Kehui Wu

研究员, 杰青  
Professor, NSFC Distinguished Young Scholar

### 研究方向 /Research Area

扫描隧道显微学, 表面科学, 低维量子材料, 分子束外延

Scanning tunneling microscopy; Surface science; Low dimension materials; Molecular beam epitaxy



赵继民  
Jimin Zhao

研究员  
Professor

### 研究方向 /Research Area

超导、强关联、拓扑等关联量子材料的超快光谱学, 超快动力学和非线性光谱学

Ultrafast spectroscopy, ultrafast dynamics; and nonlinear optical spectroscopy of correlated materials, such as superconductors, strongly correlated systems and topological materials



程鹏  
Peng Cheng

副研究员  
Associate Professor

### 研究方向 /Research Area

新型二维量子材料的分子束外延制备, 基于扫描隧道显微镜 / 扫描隧道谱的新奇物性研究

Molecular beam epitaxy of two-dimensional quantum materials; Novel electronic properties studied by low temperature STM/STS

## 实验室成员名单



冯宝杰  
Baojie Feng

副研究员  
Associate Professor

### 研究方向 / Research Area

拓扑及低维材料的电子结构研究, 分子束外延, 角分辨光电子能谱, 超快动力学

Electronic structures of topological and low-dimensional materials; Molecular Beam Epitaxy (MBE); Angle-Resolved Photoemission Spectroscopy (ARPES); Ultrafast dynamics



纪爱玲  
Ailing Ji

副研究员  
Associate Professor

### 研究方向 / Research Area

低维薄膜材料的制备及物性研究  
Fabrication and properties of low-dimension thin films



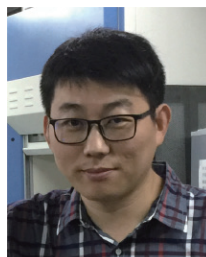
刘淼  
Miao Liu

副研究员  
Associate Professor

### 研究方向 / Research Area

材料计算模拟, 材料数据科学, 高通量计算, 能源材料

Computational materials science; Materials informatics; High-throughput computing; Energy materials



鲁年鹏  
Nianpeng Lu

副研究员  
Associate Professor

### 研究方向 / Research Area

功能性氧化物薄膜的新材料制备, 新型量子调控, 功能特性研究及模型器件的构建  
Thin film growth of newly designed complex transition metal oxides; Exploration of the exotic physical and functional properties of these materials; Fabrication of the model devices based on the discovered interesting properties with novel functionalities



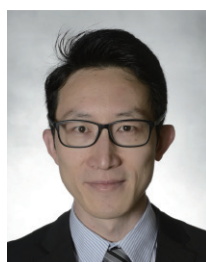
孟梦  
Meng Meng

副研究员  
Associate Professor

### 研究方向 / Research Area

低维强关联体系的外延生长, 磁性与输运性能表征, 新奇界面有序态, 物性调控

Epitaxial growth of low-dimensional strong correlated systems; Characterization of magnetism and transport properties; novel ordering states at the interface; Control of physical properties



田学增  
Xuezheng Tian

副研究员  
Associate Professor

### 研究方向 / Research Area

研究方向 / Research Area  
电子显微学, 三维原子断层成像, 凝聚态物质构效关系

Electron microscopy; 3D atomic electron tomography; Structure and properties relationships in condensed matter

# 实验室成员名单



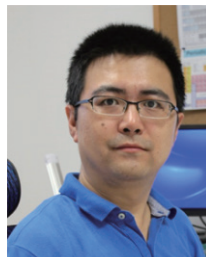
王强  
Qiang Wang

副研究员  
Associate Professor

### 研究方向 / Research Area

无序体系结构和性质研究, 体相和受限水及水溶液结构和性质, 冰形核及长大机理和调控

Structure and properties of disordered materials; Effects of size and surface properties on the structures and properties of water and aqueous solutions; Regulation of ice nucleation and growth

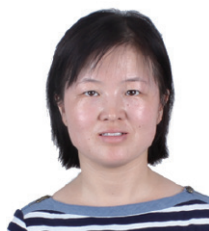


王炜华  
Weihua Wang

副研究员  
Associate Professor

### 研究方向 / Research Area

单分子与金属-有机网络, 二维材料的分子束外延生长, 扫描隧道显微学  
single molecules and metal-organic framework; molecular beam epitaxy of two-dimensional materials; scanning tunneling microscopy



王立芬  
Lifen Wang

副研究员  
Associate Professor

### 研究方向 / Research Area

原位透射电子显微学, 结构相变, 成核结晶生长动力学

In situ transmission electron microscopy; Phase transition; Nucleation and crystallization



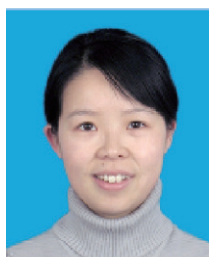
王理  
Li Wang

副研究员  
Associate Professor

### 研究方向 / Research Area

大尺寸二维单晶生长, 大尺寸金属单晶生长, 二维材料超快生长等

large-scale two-dimensional single crystal growth; large-scale metal single crystal growth; ultra-fast growth of two-dimensional materials, etc



杨芳  
Fang Yang

副研究员  
Associate Professor

### 研究方向 / Research Area

脉冲激光沉积, 过渡金属氧化物薄膜外延及其性质调控, 原子尺度精确控制

Pulsed laser deposition; epitaxy of transition metal oxide films and tuning of their properties; precise control at atomic scale



张凌云  
Lingyun Zhang

副研究员  
Associate Professor

### 研究方向 / Research Area

固体理论, 统计物理, 软凝聚态物理, 理论生物物理

Solid state theory; Statistical physics; Soft condensed matter physics; Theoretical biophysics



## 实验室成员名单



张萃  
Cui Zhang

副研究员  
Associate Professor

### 研究方向 /Research Area

表面反应机制, 极端条件下的物性特征,  
多尺度动力学模拟  
Surface reaction mechanism;  
Physical properties under extreme  
conditions; Multi-scale dynamic  
simulations



章一奇  
Yiqi Zhang

副研究员  
Associate Professor

### 研究方向 /Research Area

扫描探针显微镜, 有机小分子设计, 表面复杂结构分子晶体合成, 分子手性, 二维  $\pi$  共轭有机分子单层界面合成, 电子结构表征  
Scanning probe microscopy;  
molecular building blocks design;  
interfacial complex molecular  
tessellations; chiral molecules; on-  
surface synthesis of  $\pi$ -conjugated  
2D molecular networks; electronic  
structures characterization



朱学涛  
Xuetao Zhu

副研究员  
Associate Professor

### 研究方向 /Research Area

低维体系元激发, 电子-声子相互作用,  
高分辨电子能量损失谱, 氦原子散射  
Collective Excitations in Low-Dimen-  
sional Systems; Electron-Phonon In-  
teractions; High-resolution Electron  
Energy Loss Spectroscopy; Helium  
Atom Scattering

## 技术人员 3 名 /Technician



单欣岩  
Xinyan Shan

副主任工程师  
Senior Engineer

### 研究方向 /Research Area

超快显微光谱, 光耦合扫描隧道显微镜,  
固态纳米孔测序  
Ultrafast Spectroscopy; Photo  
assisted Scanning Tunneling Mi-  
croscope; Solid State Nanopore  
Sequencing



许智  
Zhi Xu

副主任工程师  
Senior Engineer

### 研究方向 /Research Area

透射电子显微镜原位测量技术的开发与  
应用, 精密物性测量仪器仪表的开发  
Development and application of in-  
situ TEM measurement technology;  
development of precise equipment  
and instrument for physical property  
measurement

# 实验室成员名单



李晓敏  
Xiaomin Li

副主任工程师  
Senior Engineer

### 研究方向 /Research Area

球差电镜技术及其科研应用, 原位电镜  
技术应用研究

Aberration-corrected transmission  
electron microscopy technique  
and its scientific application; In situ  
transmission electron microscopy  
technique



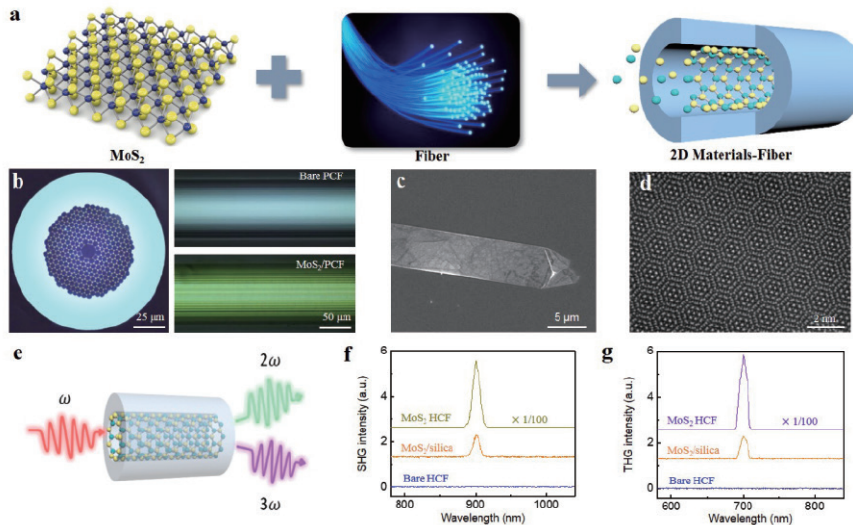
2019 年研究生考核暨学术交流大会



2020 年研究生考核暨学术交流大会

# L 实验室年度工作进展 laboratory Annual Work Progress

## 1) 制备出超高非线性二维材料复合光纤



二维材料复合光纤的制备与超高非线性光学特性

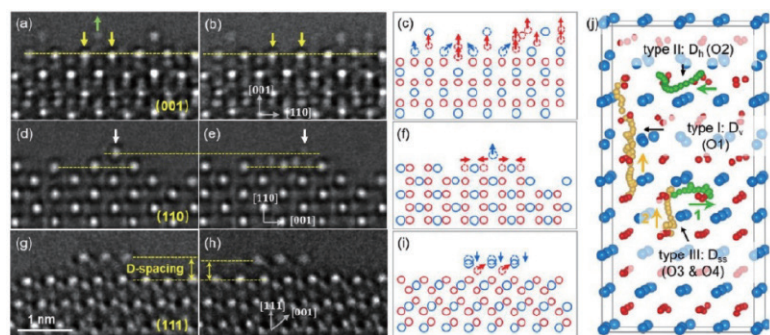
提出了一种液相辅助两步化学气相沉积法，在多孔光纤孔内壁上直接生长二维过渡金属硫族化合物，制备出具有超高非线性的二维材料复合光纤。基于该复合光纤的非线性实部和虚部分别进行了相应的应用研究：二维材料复合光纤展示了超强的二次和三次谐波产生；完成了全光纤锁模脉冲激光器的搭建和测试。[Nature Nanotech., 2020, 15:987]

### Optical fibers with embedded two-dimensional materials for ultrahigh nonlinearity

A two-dimensional (2D) material optical fiber with ultrahigh optical nonlinearity has been realized via a well designed two-step chemical vapour deposition method. Significant enhancement of second- and third-harmonic generation were realized with  $\sim 300$  times higher than that of pristine 2D materials. We also demonstrate an all-fiber mode-locked laser by integrating the 2D material optical fiber as a saturable absorber. [Nature Nanotech., 2020, 15:987]

## 2) 确定出 $\text{CeO}_2$ 晶体中氧原子的优先传输路径

利用球差校正电镜表征  $\text{CeO}_2$  晶体原子结构，实现了 Ce 原子和 O 原子直接成像，原位实验捕获反应中的氧原子和它的实时扩散路径，发现萤石结构氧化铈中氧原子以  $\langle 001 \rangle$  方向作为优先传输路径。结合第一性原理计算，揭示了二氧化铈中氧原子各向异性传输机制。[Phys. Rev. Lett., 2020, 124:056002]

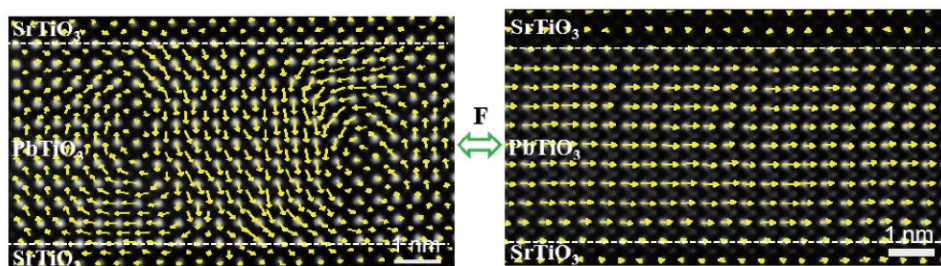


$\text{CeO}_2$  晶体氧扩散路径的电子显微学研究

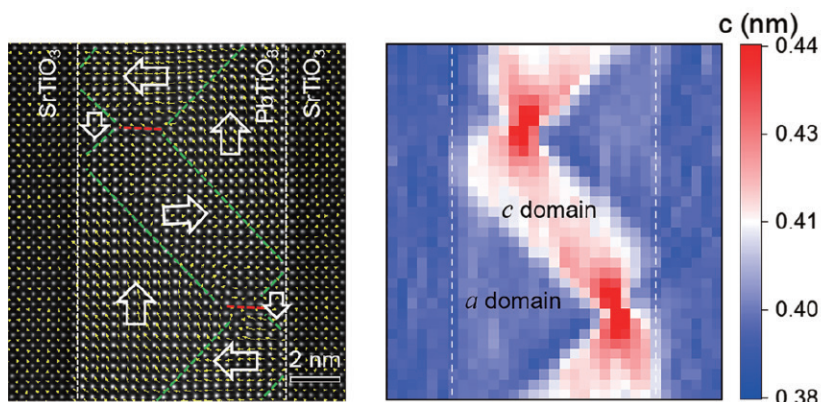
## Visualizing anisotropic oxygen diffusion path in ceria under activated conditions

Aberration-corrected transmission electron microscopy and molecular dynamics simulations were used to study the oxygen atom diffusion path in ceria under activated conditions. Reactive oxygen atom and its real-time migration were visualized. Anisotropic oxygen atom diffusion that depends on crystal orientations was discovered, demonstrating a preferential [001] crystallographic diffusion pathway. [Phys. Rev. Lett., 2020, 124:056002]

## 3) 实现了极性拓扑结构外场调控与原子尺度表征



铁电涡旋畴力场调控



极性通量闭合畴结构表征

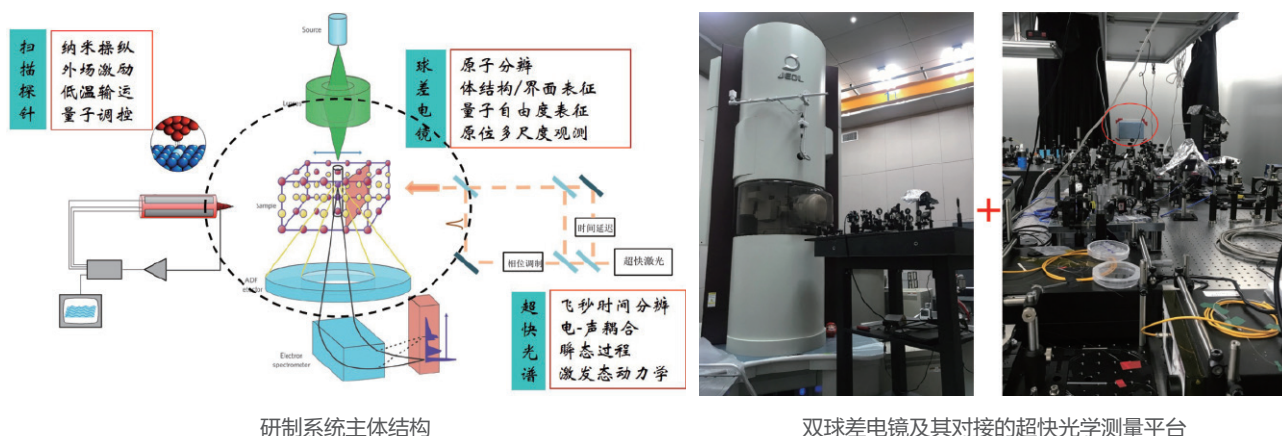
通过发展原位电镜技术，实现了铁电极性拓扑结构相变的外场操控与原子尺度表征。系统地研究了  $\text{PbTiO}_3/\text{SrTiO}_3$  超晶格中极性拓扑畴结构在外场下的动力学过程，利用原位电镜电、力局域场实现了对极性涡旋畴和通量闭合畴的操控，并借助相场模拟揭示其背后的物理机制。[Nature Commun., 2020, 11:1840; PNAS, 2020, 117:18954]

## Atomic-scale observations of manipulation of topological polar flux-closure and vortices in ferroelectric superlattice

Using atomically resolved in situ scanning transmission electron microscopy, we find that the polar flux-closures in  $\text{PbTiO}_3/\text{SrTiO}_3$  superlattice films are mobile and can be reversibly switched to ordinary single ferroelectric c- or a-domains under an applied electric field or stress. And the vortices undergo a transition to the a-domain under external compressive stress. These processes are reproduced by using phase-field simulations. [Nature Commun., 2020, 11:1840; PNAS, 2020, 117:18954]

# 实验室年度工作进展

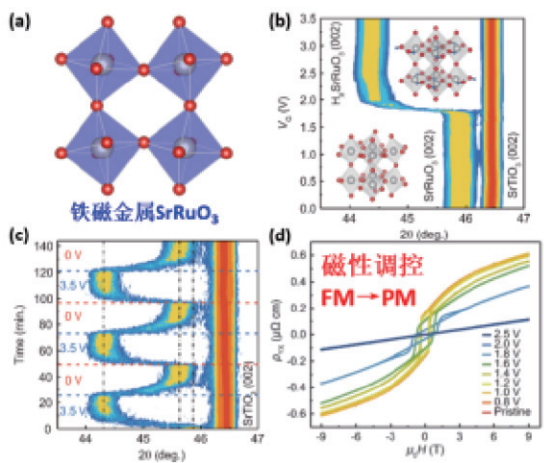
## 4) 成功研制超高时空分辨原位电镜多尺度量子测量系统



发挥利用球差电镜、扫描探针、超快光谱技术特长，在球差电镜中搭建完成超高时空分辨综合物性测量系统，具有低温扫描探针输运测量与多场量子调控以及超快光谱测量功能，达到原子分辨和百飞秒时间分辨物理测试能力。[Rev. Sci. Instrum., 2021, 92:013704]

By taking advantage of aberration-corrected transmission electron microscopy, scanning probe and ultrafast optical spectroscopy technique, an ultrahigh space- and time- resolution physical measurement system has been built, which can perform the low-temperature transport and ultrafast optics experiments, and the related quantum manipulation can also be carried out by the external multi-fields. The performance of this system reaches atomic-level space resolution and hundreds-femtosecond time resolution. [Rev. Sci. Instrum., 2021, 92:013704]

## 5) 氧化物离子调控及物性研究



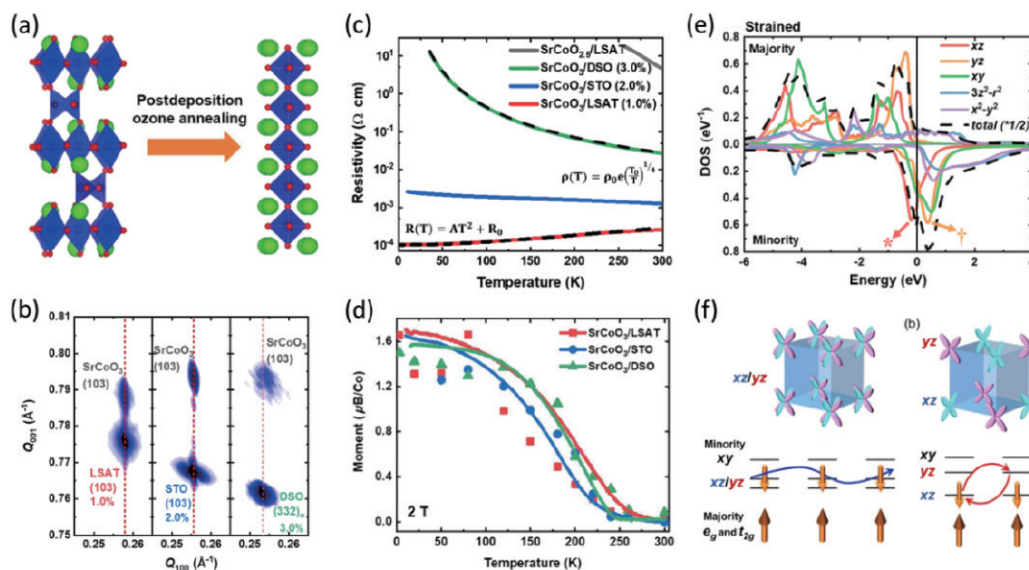
电场控制 H<sup>+</sup> 离子嵌入实现 SrRuO<sub>3</sub> 材料磁性调控

利用离子调控的方法实现了电场对铁磁金属 SRO 铁磁性及拓扑相变的控制。通过电场控制的离子调控，他们实现了：(1) 质子嵌入使 SRO 晶格在 c 方向发生了 3.3% 的膨胀；(2) 质子的嵌入使 SRO 发生了从铁磁到顺磁的相变；(3) 质子嵌入造成的浓度梯度使 SRO 晶格空间反演对称破缺，再结合 D-M 相互作用，最终实现了电场对拓扑霍尔效应的调控。该研究成果于 2019 年 12 月被《自然-通讯》杂志接收 (Nat. Commun. 11, 184 (2020))。

Using the ferromagnetic metal SrRuO<sub>3</sub> as a model system, we demonstrate an efficient and reversible control of both structural and electronic phase transformations through the electric-field controlled proton evolution with ionic liquid

# 实验室年度工作进展

gating. The insertion of protons results in a large structural expansion and increased carrier density, leading to an exotic ferromagnetic to paramagnetic phase transition.



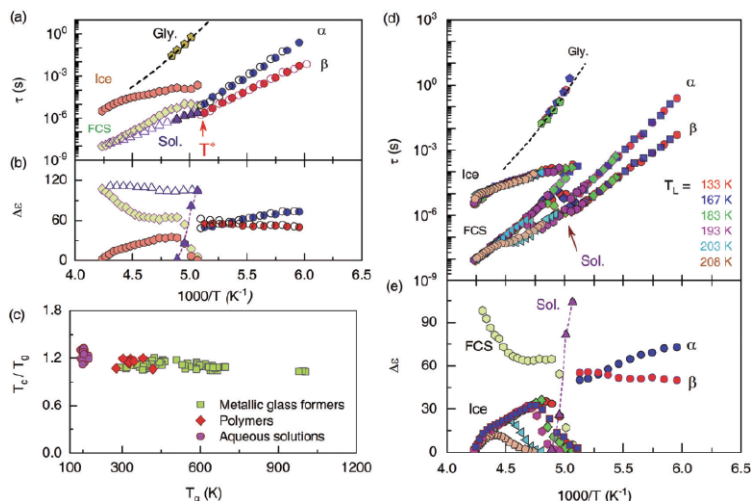
钙钛矿结构钴酸锶高拉伸应力下的磁电特性演化及磁性机理研究

通过臭氧退火的方法，制备了钙钛矿结构的  $\text{SrCoO}_3$  (图 a)，其具有严格的外延特性和极高的结晶质量 (图 b)。对其进行磁、电输运测量，发现随着应力增大，会发生从金属到绝缘体的转变 (图 c)，而铁磁性则始终保持 (图 d)。相关成果于 2020 年 3 月份发表在 PRX 上 (Phys. Rev. X 10, 021030 (2020))。

Using a postdeposition ozone annealing method, we obtain a series of oxygen stoichiometric  $\text{SrCoO}_3$  thin films with the tensile strain up to 3.0%. We observe a robust ferromagnetic ground state in all strained thin films, while interestingly the tensile strain triggers a distinct metal-to-insulator transition along with the increase of the tensile strain.

## 6) 水溶液的玻璃化及冷结晶

主要揭示了深过冷、低水含量、慢扩散的条件下局域结合水和自由水完全参与冰冷结晶的中间过程；冷结晶结束后溶质周围即均被不参与冷结晶的结合水包围。相关成果于 2019 年 4 月份发表在 Phys.Chem.Chem. Phys. 上 (Phys.Chem.Chem.Phys.21,10293 (2019))。



甘油水溶液中冰冷结晶前后结合水和自由水介电弛豫时间与温度关系

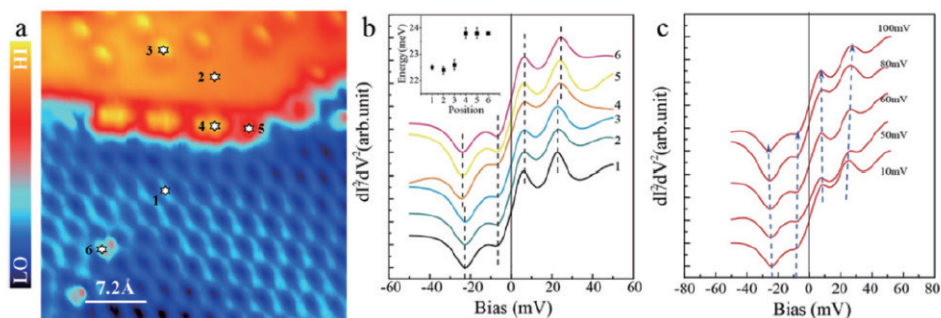
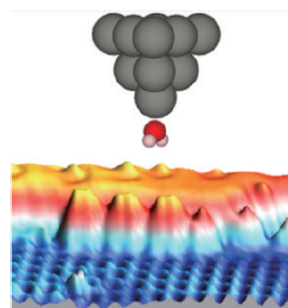
## 实验室年度工作进展

Under the conditions of deeply supercooled state, low water content, and slow diffusion, bound water and free water can both participate in the process of ice nucleation. This can compensate for the effect of low diffusion of water in deeply supercooled condition (see Phys.Chem.Chem.Phys.21,10293 (2019)).

### 7) 表面激发态超快动力学过程的探测研究

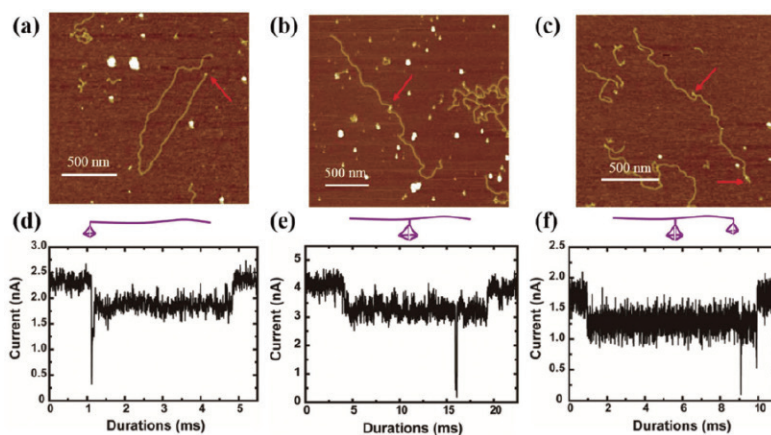
研究半导体 GaAs 表面单个缺陷的光生载流子复合过程超快动力学; 利用非弹性隧穿研究了单个水分子的转动和振动激发 [J. Phys. Chem. Lett. 2020, 11, 1650-1655]。

We demonstrate the measurement of transient photo-excited carrier dynamics on GaAs(110) surface by time-resolved scanning tunneling microscopy. Time-resolved  $dI/dV$  spectra were carried out on GaAs (110) surface and on a single Arsenic vacancy defect. Using inelastic electron tunneling spectroscopy, two low-energy excitations of a single water molecule are observed, where a significant enhancement is achieved by attaching the molecule to the tip apex in a scanning tunneling microscope.



### 8) 纳米孔 DNA 测序技术的研究

研究了 DNA 折纸四面体在固态纳米孔中的穿孔过程 ([Nanoscale, 11, 6263-6269 (2019)]); 制备了绝缘的纳米孔支撑结构; 开发了纳米孔测序序列比对的程序, 获得了解旋酶对四种碱基的特异性差分力谱。



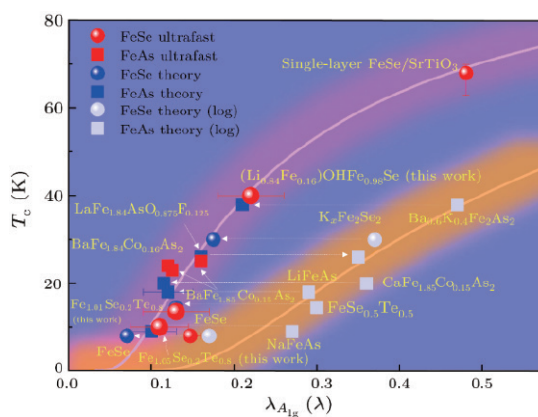
## 实验室年度工作进展

Tetrahedral DNA nanostructures (TDNs) are programmable DNA nanostructures that have great potential in bio-sensing, cell imaging and therapeutic applications. We investigate the translocation behavior of individual TDNs through solid-state nanopores. Pronounced translocation signals for TDNs are observed that are sensitive to the size of the nanostructures.

Revealing complex interactions between DNA and motor proteins at the microscopic level is important for understanding the nature of life. We utilized the advantage of highly parallel nanopore DNA sequencing by MinION to explore the kinetics that were not possible to be detected before. By examining the correlation between translocation dwell time and the sequence, we obtained differential interaction forces between each DNA base and the protein.

9) 研究了  $(\text{Li}_{0.84}\text{Fe}_{0.16})\text{OHFe}_{0.98}\text{Se}$  等铁基高温超导的电-声子耦合, 发现了铁基超导体里普遍存在的  $T_c$  与 EPC 强度  $\lambda_{A_{1g}}$  或  $\lambda$  之间的正相关关系。 (CPL (Express Letter) 37, 097802 (2020))。

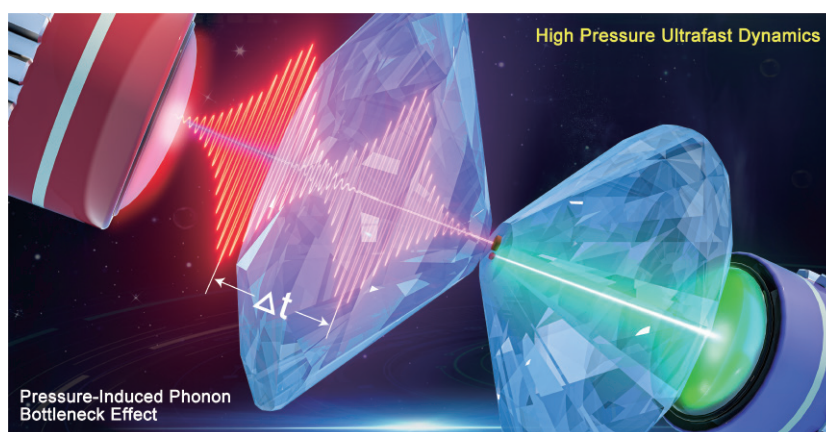
We investigated the electron-phonon coupling in  $(\text{Li}_{0.84}\text{Fe}_{0.16})\text{OHFe}_{0.98}\text{Se}$ . Discovered a universal positive correlation between  $T_c$  and the e-phonon coupling strength  $\lambda_{A_{1g}}$  or  $\lambda$  for all types of optimally doped iron-based superconductors, including the monolayer ones.



10) 研究了强关联氧化物  $\text{Sr}_2\text{IrO}_4$  的高压超快动力学并发现了压强诱导的声子瓶颈效应, 研究了外尔半金属 TaAs、三重简并拓扑半金属 MoP、节线拓扑绝缘体 LaBi 的超快动力学及相干态声子等 [CPL (Express Letter) 37, 047801 (2020), Phys. Rev. Materials 4, 064201 (2020), Opt. Express 28, 15855 (2020)].

We investigated the high-pressure ultrafast dynamics in  $\text{Sr}_2\text{IrO}_4$  and discovered pressure-induced phonon bottleneck effect.

Investigated the ultrafast dynamics and coherent phonon in Weyl semimetal TaAs, triple degenerate topological semimetal MoP, and nodal-line topological material LaBi [CPL (Express Letter) 37, 097802 (2020), CPL (Express Letter) 37, 047801 (2020), PR Materials 4, 064201 (2020), Opt. Express 28, 15855 (2020)].





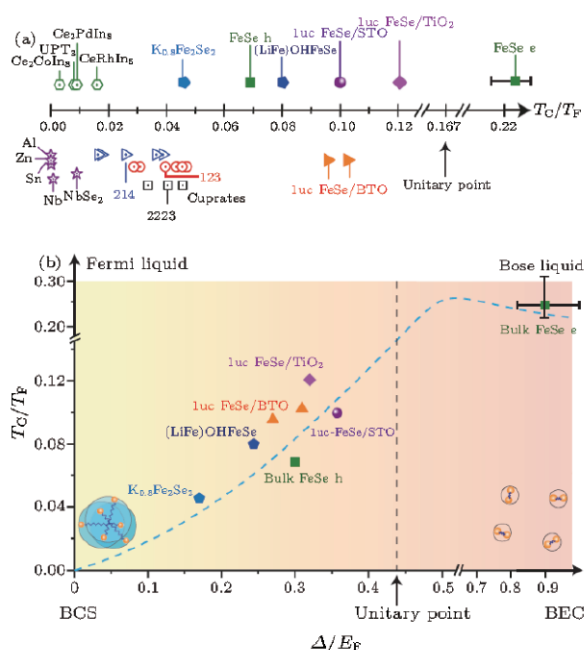
## 实验室年度工作进展

11) 利用 BCS-BEC 相图分析了 FeSe/SrTiO<sub>3</sub> 超导增强界面的特殊性: FeSe 与其它超导材料相比更接近 crossover 区, 灵敏地响应衬底引入的修饰作用。进一步利用有机分子吸附对载流子浓度的降低作用, 可以驱动体系在 BCS-BEC 相图中的演化, 并直接观察到电子预配对的特征。

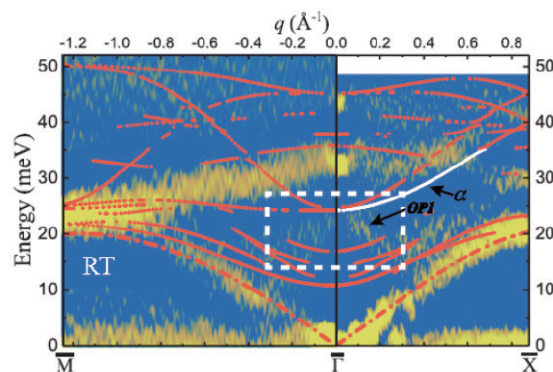
We described the uniqueness of the FeSe/SrTiO<sub>3</sub> interface with superconductivity enhancement in the BCS-BEC phase diagram: FeSe is closer to the crossover region than any other known superconductors, and therefore responds sensitively to the modifications introduced by the substrate. We further drive the evolution of the system in the BCS-BEC phase diagram by reducing the carrier density associated with the surface adsorption of semiconducting molecules. The pseudogap phase was detected by the scanning tunneling microscopy.

12) 测量了拓扑节线半金属 ZrSiS 表面的声子色散谱, 发现一支表面光学声子在各高对称方向均具有显著的能量软化特征, 这起源于表面光学支声子与 ZrSiS 新奇二维表面态之间的相互作用。

By the precise measurements of the surface phonon dispersions of the topological nodal-line semimetal, ZrSiS, we observed the softening behaviors along all the high-symmetry directions, which originate from the coupling with the special surface states.



Shuyuan Zhang, Guangyao Miao, Jiaqi Guan, Xiaofeng Xu, Bing Liu, Fang Yang, Weihua Wang, Xuetao Zhu, Jiandong Guo, Superconductivity of the FeSe/SrTiO<sub>3</sub> Interface in the View of BCS-BEC Crossover, *Chin. Phys. Lett* 36, 107404 (2019).

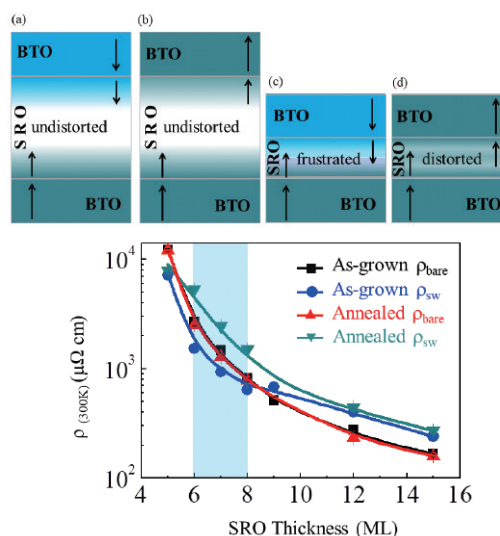


Siwei Xue, Tiantin Zhang, Changjiang Yi, Shuyuan Zhang, Xun Jia, Luiz H. Santos, Chen Fang, Youguo Shi, Xuetao Zhu, and Jiandong Guo, Electron-Phonon Coupling and Kohn Anomaly due to the Floating 2D Electronic Bands on the Surface of ZrSiS, *Phys. Rev. B* 100, 195409 (2019).

## 实验室年度工作进展

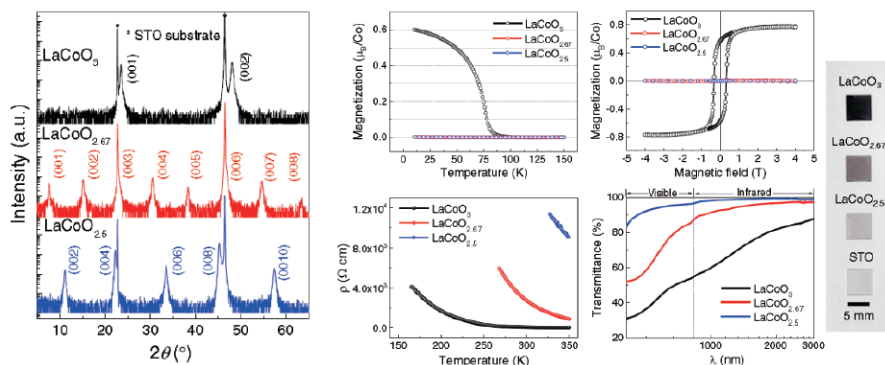
13) 制备了  $\text{BaTiO}_3/\text{SrRuO}_3/\text{BaTiO}_3$  三明治结构并控制两侧铁电 BTO 层平行 / 反平行取向, 在适当中间非铁电 SRO 层厚度的结构中获得了 250% 的电阻变化。

We prepared the sandwich structure of  $\text{BaTiO}_3/\text{SrRuO}_3/\text{BaTiO}_3$  and controlled the ferroelectric orientation of the BTO layers. In the structure with suitable SRO thickness, the resistance varied by a ratio up to 250%.



Qing Zhu, Fang Yang, and Jiandong Guo, Coupling of polarization orientations of the ferroelectric layers sandwiching a metal film, Appl. Phys. Lett. 116, 181602 (2020).

14)



Qichang An, Meng Meng, Zhenzhen Wang, Yade Wang, Qinghua Zhang, Yuxuan Xia, Lin Gu, FangYang, and Jiandong Guo, Realization of Monophased  $\text{LaCoO}_x$  Films with Ordered Oxygen Vacancies, Physica Status Solidi A: Applications and Materials Science 217, 1900848 (2020).

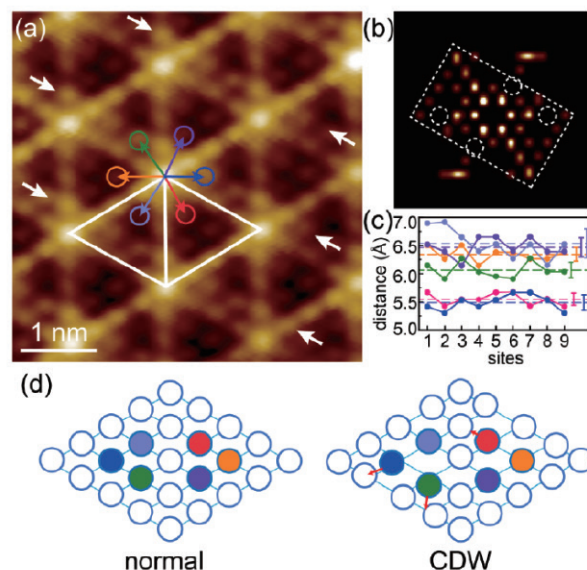
对  $\text{SrTiO}_3$  衬底外延的  $\text{LaCoO}_3$  薄膜, 利用特殊的退火方法抑制衬底向薄膜供氧, 从而可控制得到大面积均匀单相的  $\text{LaCoO}_{2.67}$  和  $\text{LaCoO}_{2.5}$  薄膜, 相应观测到薄膜电、磁、光学性质的变化。

We annealed the  $\text{LaCoO}_3$  film epitaxially grown on  $\text{SrTiO}_3$  by a special technique that suppressed the oxygen diffusion from the substrate. Uniform, monophased  $\text{LaCoO}_{2.67}$  and  $\text{LaCoO}_{2.5}$  films were obtained under control. The corresponding responses of the electric, magnetic, optical properties were measured.

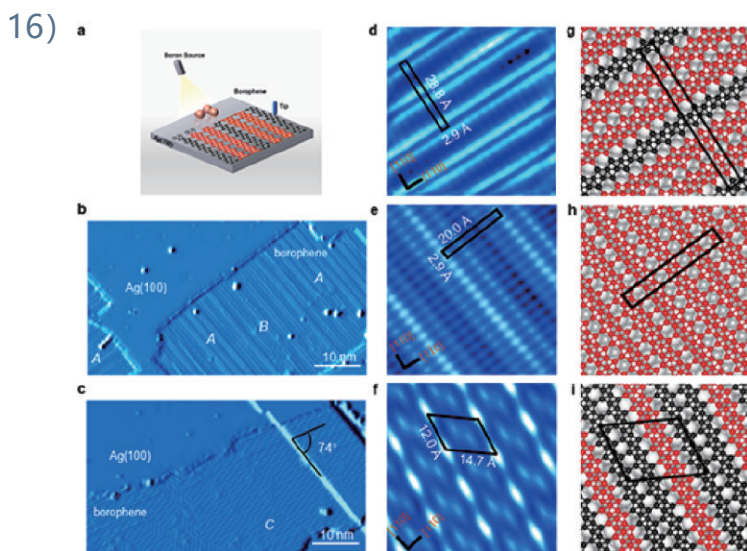
## 实验室年度工作进展

15) 制备了单层  $\text{VTe}_2$  薄膜并且观测到与  $(4 \times 4)$  电荷密度波共存的一维结构调制, 表明在被一般认可的费米面嵌套图像之外, 该体系还存在能够打破其旋转对称性的其他物理机制。

We grew monolayered  $\text{VTe}_2$  film and observed the one-dimensional structure modulation coexisting with the  $(44)$  charge-density wave. It is revealed that, beyond Fermi surface nesting, there exists the physical mechanism breaking the rotational symmetry of the system.



Guangyao Miao, Siwei Xue, Bo Li, Zijian Lin, Bing Liu, Xutao Zhu, Weihua Wang, and Jiandong Guo, Real-space investigation of the charge density wave in  $\text{VTe}_2$  monolayer with broken rotational and mirror symmetries, *Phys. Rev. B* 101, 035407 (2020).



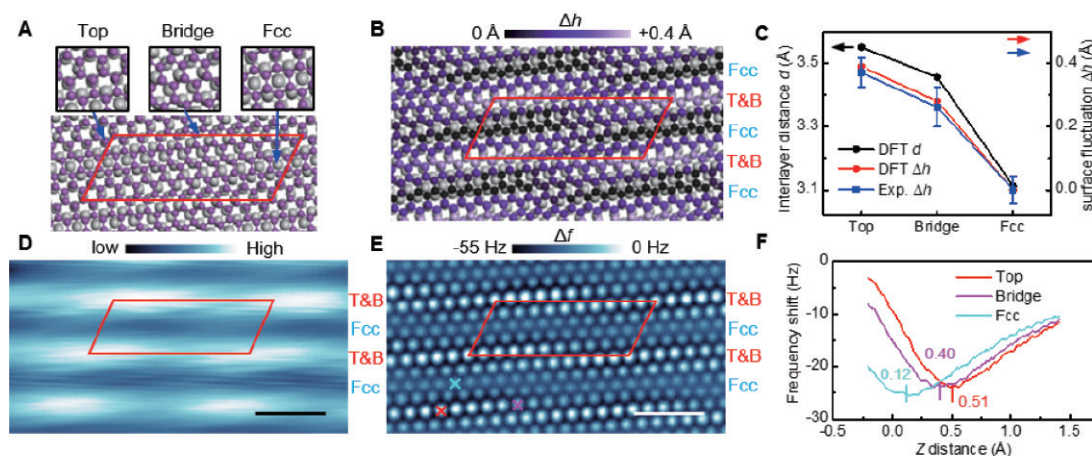
在  $\text{Ag}(100)$  衬底上利用 MBE 技术生长的单原子层厚度的混合相硼烯。(a) 是示意图。(Advanced Materials 的 Table of Contents 图)。(b-c) 是  $\text{Ag}(100)$  上硼烯岛的扫描隧道显微镜图(微分图)。(d-f) 是三种硼烯相的高分辨扫描隧道显微镜图, (g-i) 是对应的三种硼烯相的原子结构模型, 其中, A 相 (g) 和 C 相 (i) 是典型的准一维原子链混合相结构。

实验可控合成有序的准一维硼烯链混合相: 利用分子束外延 (MBE) 方法, 在  $\text{Ag}(100)$  单晶表面成功获得了两种不同的硼烯长程有序相结构。实验中获得这两种硼烯相是由两种不同种类的硼链 [(2, 3) 链和 (2, 2) 链] 通过不同的固定比例混合而成的长程有序相, 并且可以根据衬底的晶体方向得到很好的分离。通过扫描隧道显微镜表征并结合第一性原理计算, 我们揭示了混合链相的形成是由硼烯结构单元与  $\text{Ag}(100)$  表面界面相互作用所调制的, 其晶格匹配以及硼链相对于衬底的取向对这两种混合相的形成起着至关重要的作用。该结果发表在 *Adv. Mater.* 2020, 32: 2005128。

Due to a substrate mediation effect, artificial long-range ordered phases of borophene consisting of different combinations of boron chains seamlessly

joined together can be achieved on Ag(100). Scanning tunneling microscopy measurements and theoretical calculations reveal that mixed-chain phases are more stable than the pure phase, and interact only weakly with the substrate. The mixed-chain phases with various proportions of different chains can be well separated based on the crystal direction of the substrate. This work is published in *Adv. Mater.* 2020, 32: 2005128.

17)



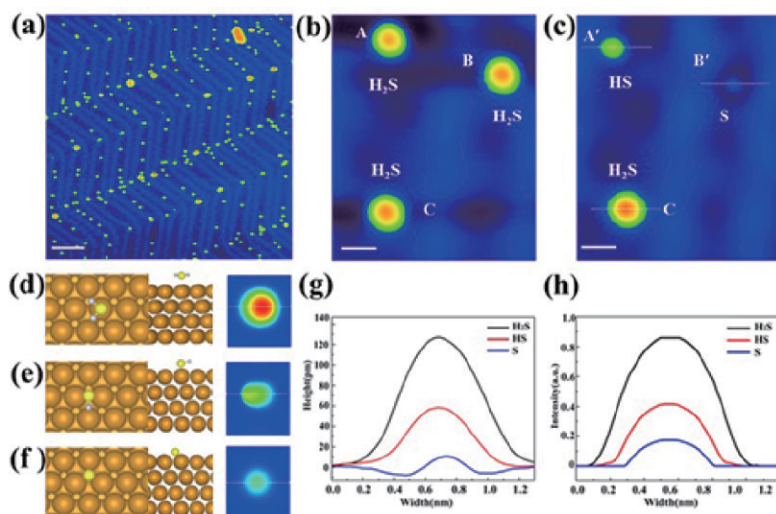
铋烯 / 类黑磷铋结构的结构特征计算 (A-C) 以及实验精确测量 (E-F)

铋烯同质结中莫尔超周期对拓扑边缘态的调制：利用分子束外延技术在高定向热解石墨（HOPG）表面获得了铋的单层的类黑磷结构相（BP-Bi）以及单层的蜂窝状铋烯相（Bismuthene）。两种单层结构相在垂直方向堆叠形成铋烯 / 类黑磷铋（Bismuthene/BP-Bi）的同质结，由于其层间的对称性差异（铋烯属于六角晶格而类黑磷铋是长方形晶格），促成了莫尔超结构的形成。通过扫描隧道显微镜 / q-plus 原子力显微镜的研究，发现莫尔周期对单层铋烯的拓扑边缘态具有调制的作用，该结果发表在 *Science Advances* 2020, 6: eaba2773。

Bismuth homostructure consisting of monolayer bismuthene and single-layer black phosphorus-like Bi (BP-Bi) was successfully grown on HOPG. Combining STM/STS with noncontact atomic force microscopy, moiré superstructures with twist angles in the bismuth homostructure and the modulation of topological edge states of bismuthene were observed. First-principles calculations indicated that the structure fluctuation is ascribed to the stacking modes between bismuthene and BP-Bi, which induce spatially distributed interface interactions in the bismuth homostructure. The paper is published in *Science Advances* 2020, 6: eaba2773 (2020).

## 实验室年度工作进展

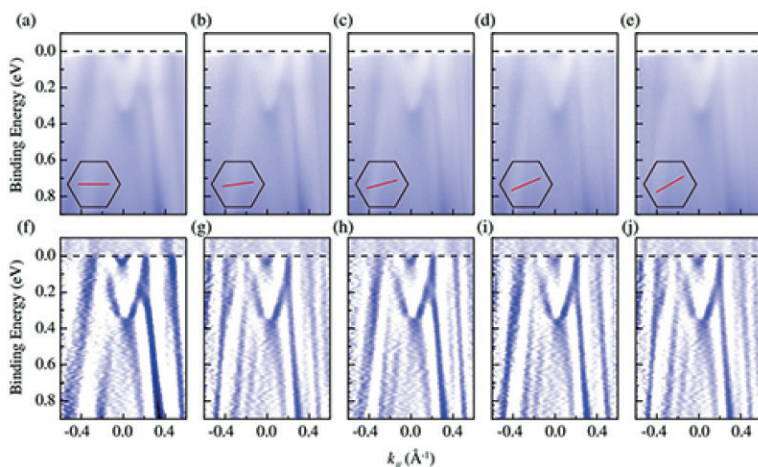
18) 利用选择性振动激发实现单分子解离反应的动力学研究：利用扫描隧道显微镜在 Au(111) 表面实现了单个 H<sub>2</sub>S 分子的解离，利用隧穿电子。实验研究和理论计算相结合的结果表明，隧穿电子促使分子振动被选择性激发，诱导了 H-HS 和 H-S 的化学键断裂。结合非绝热动力学模拟，我们从时间尺度上理解了隧穿电子以及分子的振动激发诱导解离的整个动力学过程，并在定量上发现了分子在表面的解离概率与分子激发态的寿命直接关联。该工作发表在 Phys. Rev. Lett. 2019, 123: 246804。



H<sub>2</sub>S, HS, S 在 Au (111) 表面的形貌以及模拟的结构模型

We demonstrate H – HS and H – S bond breaking on Au(111) induced by tunneling electrons using low-temperature STM. An experimental study combined with theoretical calculations shows that the dissociation pathway is facilitated by vibrational excitations. Combined with time-dependent ab initio non-adiabatic molecular dynamics simulations, the dynamics of the injected electron and the phonon-excitation-induced molecule dissociation can be understood at the atomic scale, demonstrating the potential application of STM for the investigation of excited-state dynamics of single molecules on surfaces. This work is published in Phys. Rev. Lett. 2019, 123: 246804.

19) 在一种单层铁磁材料中发现外尔节线：通过利用同步辐射角分辨光电子能谱 (ARPES) 并结合理论计算，我们在一种单原子层的铁磁材料 GdAg<sub>2</sub> (T<sub>c</sub> ≈ 85 K) 中，发现了自旋极化的外尔节线。通过深入的分析发现这些外尔节线受到晶体对称性的保护，因此具有很好的稳定性。另外，单层 GdAg<sub>2</sub> 中的某些外尔节线会随着磁化方向的不同而选择性地打开能隙。该研究成果发表在 Phys. Rev. Lett. 2019, 123: 116401。

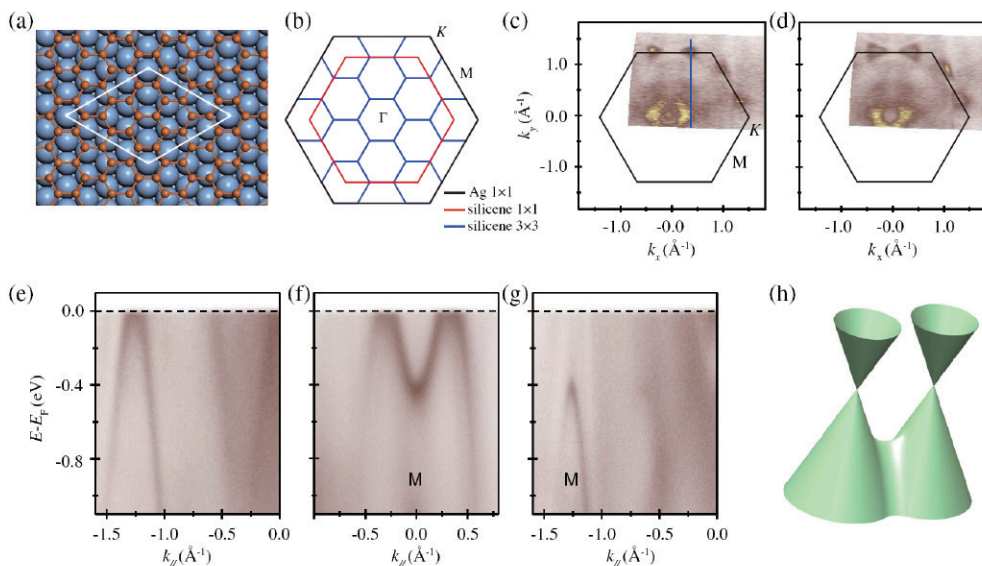


ARPES 测量结果：证实 GdAg<sub>2</sub> 中存在外尔节线

## 实验室年度工作进展

We discovered of twofold degenerate Weyl nodal lines in a 2D ferromagnetic material, a single-layer gadolinium-silver compound, based on combined angle-resolved photoemission spectroscopy measurements and theoretical calculations. These Weyl nodal lines are symmetry protected and thus robust against external perturbations. The coexistence of magnetic and topological order in a 2D material is likely to inform ongoing efforts study the rich physics in 2D topological ferromagnets. This work is published in Phys. Rev. Lett. 2019, 123: 116401.

20)



硅烯的原子结构及成对出现的狄拉克锥

硅烯中发现周期势诱导的狄拉克锥的劈裂：利用同步辐射光源的 ARPES 详细地研究了硅烯的电子结构，利用线二色性效应，发现狄拉克锥仅对 p 偏振光可见，结合 ARPES 中的矩阵元效应，可以判断出这些狄拉克锥主要来自于硅的 pz 轨道，从而在实验上证实了这些狄拉克锥来自于硅烯本身。利用第一性原理及紧束缚模型，他们发现硅烯与衬底形成的  $4 \times 4$  超结构将产生周期性的势场，该周期势场将使狄拉克锥发生劈裂。这项工作一方面为调控狄拉克锥的物性提供了一项重要的手段，另一方面澄清了长期以来硅烯中的狄拉克锥是否被衬底破坏的争议。这一成果发表在 Phys. Rev. Lett. 2019, 122: 196801 上。

We studied the electronic structures of  $(3 \times 3)$ -silicene on Ag(111) using high-resolution ARPES and confirmed the existence of six pairs of Dirac cones at the BZ boundary of Ag(111). These Dirac cones were only detectable with p polarized light, indicating that the Dirac bands are mainly derived from the pz orbitals of silicon. Our tight-binding analysis and DFT calculations revealed that these Dirac cones originate from the original Dirac cones of freestanding silicene. Our results settle the long-debated question on the existence of Dirac cones in the silicene/Ag(111) system, and provide a powerful route to tailor the physical properties of Dirac fermions in a honeycomb lattice. This work is published in Phys. Rev. Lett. 2019, 122: 196801.

## 实验室年度工作进展

21)



Some software based on rt-TDDFT and their main features

	TDAP	TDAPW	OCTOPUS	ELK	GPAW	YAMBO	NWCHEM	SALMON
Dipole Field	✓	✓	✓	•	✓	•	✓	✓
Vector Field	✓	✓	✓	✓	×	✓	×	✓
Berry Phase	✓	×	×	✓	×	✓	×	×
MD	✓	✓	✓	×	•	×	•	•
PIMD	✓	✓	×	×	×	×	×	×
TypeBasis	NAO <sup>2</sup>	PW <sup>3</sup>	RSG <sup>3</sup>	PW <sup>4</sup>	RSG/NAO	RSG	Gaussian	RSG <sup>3</sup>
NumBasis/N <sub>e</sub>	10	10 <sup>3</sup>	10 <sup>4</sup>	10 <sup>5</sup>	10 <sup>5</sup> /10	10 <sup>4</sup>	10 <sup>2</sup>	10 <sup>4</sup>
TimeStep/as	50	50	1	1	10	1	2.5	1

[✓: Realized] [•: Realized but problematic] [×: Not realized]

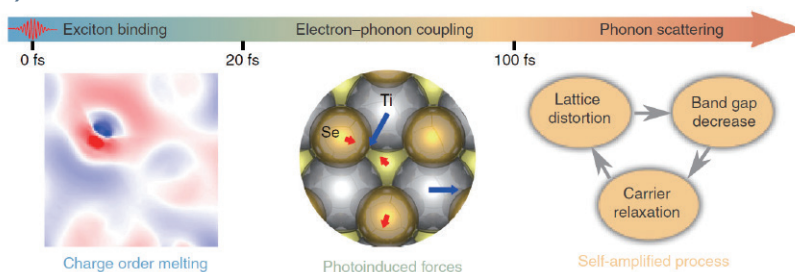
“First-principles dynamics of photoexcited molecules and materials towards a quantum description”, WIREs: Compu. Mol. Sci. 2021,11:1492.

has unique features and advantages compared to other such computational packages. The development and application of this method represents an important progress in the study of full quantum dynamics of electrons and nuclei from first-principles, allowing us to obtain a complete and predictable understanding of quantum interactions and dynamic processes in complex condensed matter systems from the microscopic level.

实现了包含电子激发效应和核量子效应的凝聚态多维体系的全量子化动力学模拟，自主开发的非绝热激发态计算模拟软件 (TDAP/TDAPW) 具有同类计算软件所不具备的特色和优势。此方法的发展和應用代表了从第一性原理出发研究电子和原子核的全量子动力学的重要进展，使得我们可以从微观层面上对复杂凝聚态体系中的量子相互作用和动力学过程有一个完整和可预测的理解。

We achieved full quantum first-principles description of condensed multi-dimensional system, including electronic excitation and nuclear quantum effects. The self-developed nonadiabatic excited-states simulation software (TDAP/TDAPW)

22)



“Ultrafast charge ordering by self-amplified exciton-phonon dynamics in TiSe<sub>2</sub>”, Nature Comm. 2020, 11:43.

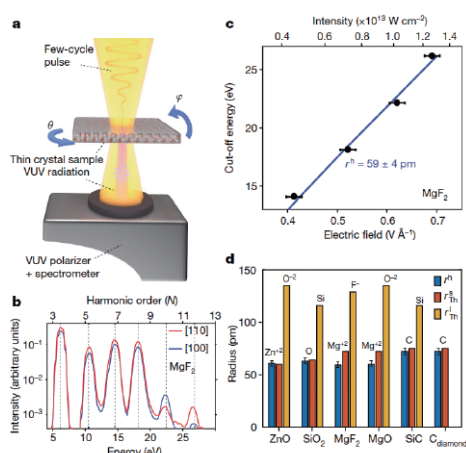
对激光激发二硒化钛的超快动力学进行了同时具有超快时间分辨和原子精度空间分辨的第一性原理研究，发现了其电荷密度波形成的激子-声子的自放大机制。我们观测到这一过程的时间尺度约为 100 飞秒，与含时角分辨电子谱的实验测量一致。这为研究电荷密度波的形成机理提供了新的研究思路。 [Nature Comm. 2020, 11:43.]

We completed the first-principles study on the ultrafast dynamics of laser-excited TiSe<sub>2</sub> with ultrafast time resolution and atomic spatial resolution, and discovered the ultrafast charge ordering in TiSe<sub>2</sub> by self-amplified exciton-phonon dynamics. We observed that the time scale of this process is about 100 fs, which is consistent with the time-resolved and angle-resolved photoemission spectroscopy measurements. It provides a new way to study the formation mechanism of charge density wave.

## 实验室年度工作进展

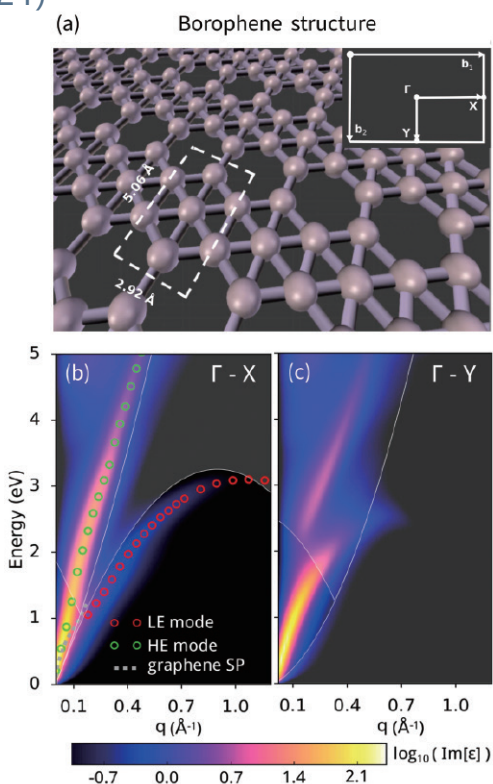
23) 与实验研究人员合作，利用高次谐波实现了固体中皮米 ( $10^{-12}$  m) 精度的价电子势能和密度的空间成像，开发了一种能够探测价电子密度的新型光显微镜，使得我们能够以前所未有的分辨率捕捉微观世界的细节。[Nature 2020, 583:55]

In cooperation with experimentalists, we realized the spatial imaging of valence electron potential energy and density with Pico meter ( $10^{-12}$  m) accuracy by using high-order harmonics, and developed a new optical microscope to detect the density of valence electrons, which enables us to capture the details of the micro world at unprecedented resolution.



“Laser picoscopy of valence electrons in solids” ,  
Nature 2020, 583:55.

24)



“Integrated plasmonics: broadband Dirac plasmons in borophene” , Phys. Rev. Lett., 2020, 125:116802.

通过对硼烯的集体激发探究，揭示了在硼烯中存在奇异的量子等离激元行为。各向异性的一维等离激元起源于硼烯中倾斜狄拉克锥的电子跃迁，类似于极端掺杂石墨烯中的电子跃迁。这些特性使硼烯成为一维、二维和狄拉克等离激元的集成平台，有希望在下一代光电器件中实现定向极化传输和宽带光通信。[Phys. Rev. Lett., 2020, 125:116802]

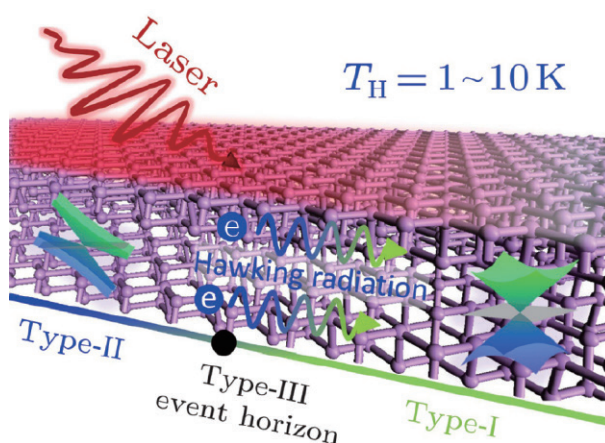
We studied the collective excitations in borophene and revealed the integrated quantum plasmon behaviors in borophene. The anisotropic 1D plasmon originates from electronic transitions of tilted Dirac cones in borophene, analogous to that in extreme doped graphene. These features enable borophene as an integrated platform of 1D, 2D, and Dirac plasmons, promising for directional polariton transport and broadband optical communication in next-generation optoelectronic devices.



## 实验室年度工作进展

25) 利用第一性原理量子激发动力学计算和量子隧穿模型分析, 我们预言了光场辐照下黑磷中的费米子高温霍金辐射。这个系统呈现出迄今为止最高、且实验可探测的霍金温度 ( $1 \sim 10 \text{ K}$ )。[Chin. Phys. Lett. (Express Letters) 2020,37:067101]

Using first-principles quantum excitation dynamics calculation and quantum tunneling model analysis, we predicted the high temperature fermion Hawking radiation in black phosphorus. This system presents so far the highest and experimentally detectable Hawking temperature ( $1 \sim 10 \text{ K}$ ).



"Fermionic analogue of high temperature Hawking radiation in black phosphorus", Chin. Phys. Lett. 2020,37:067101

26) 完成第一原理材料数据库 (Atomly.net) 和高通量计算平台的建设。Atomly.net 致力于开创世界级材料基因工程知识库。运用业界顶级的材料数据科学技术将 17 万 + 个无机材料的高质量数据带给你触手可得之处。Atomly 为业界带来材料数据工具平台, 通过数据驱动新材料的筛选、预测和发现, 提升材料研发的生产力。

Complete the building of first-principles materials database (Atomly.net) and high-throughput computing platform. Atomly.net is a world-class materials genome knowledge-base to bring the state-of-art materials science high-quality data to your fingertips. Atomly provides a revolutionary data-driven infrastructure to the materials science community, hence people could screen, predict, and discover new materials in an expedite and cost-effective manner.



## 表面科学论坛邀请报告

序号	报告人	报告题目	机构
1	Martin Wenderoth	Charge Dynamics at Semiconductor Surfaces Investigated by Time Resolved Scanning Tunneling Microscopy	Georg-August-University of Göttingen
2	Jianhui Zhou	Novel Plasmons in Quantum Anomalous Hall Insulators	High Magnetic Field Laboratory, Chinese Academy of Sciences
3	Yiqi Zhang	Recent advances in on-surface chemistry of alkyne derivatives: novel reactions and functional architectures	Physics Department, Technical University of Munich
4	Libo Ma	Self-assembled microtubular cavities as a platform for surface sensing	Institute for Integrative Nanosciences, IFW Dresden
5	Yifei Mo	Computation Accelerated Design of Materials and Interfaces for Solid-state Batteries	University of Maryland, College Park
6	Yang Chai	Multifunctional Electronic Devices Based on Transition Metal Oxide	The Hong Kong Polytechnic University
7	Katsuo Tsukamoto	Recent Progress on In-Situ Observations of Crystal Growth from Liquids at Atomic Level	Tohoku University/Osaka University/Nagoya University, JAPAN
8	Hrvoje Petek	How to dress a metal	University of Pittsburgh
9	Chongqin Zhu	水在界面的结构、动力学和浸润性	University of Pennsylvania
10	Di Yi	3d/5d 过渡金属氧化物异质结构的新颖物性及调控	Tsinghua University
11	Xusheng Cai	等离子体 / 离子束辅助制备二维纳米材料	Harbin Institute of Technology

### 表面物理半月谈

序号	报告人	报告题目
1	余博哈	时间分辨的透射电镜
2	赵新佳	固 - 液界面的基本物理问题—电双层及 zeta 势
3	徐小凤	Light-induced/enhanced superconductivity
4	苗光耀	电荷密度波的一些事儿
5	张嘉翔	二维铁电与磁电耦合
6	申钰田	Nonlinear optical spectrums of water
7	刘新豹	Valley polarized excitons in the atomically thin transition metal dichalcogenides
8	张和煦	Q-Plus AFM and its Application
9	李淑荟	Quantum Anomalous Hall Effect –from magnetic-doping TIs to intrinsic magnetic materials (TIs or WSMs)
10	李轩熠	物理学和计算机
11	游佩桅	Hubbard U in First principles Calculation
12	王 恩	Introduction of Driven Quantum System
13	李 博	Introduction of Spin-Polarized Scanning Tunneling Microscopy
14	宋晨晨	Modulation of ferroelectricity in materials by ultrafast lasers

主办国际会议



  
中国科学院物理研究所  
Institute of Physics Chinese Academy of Sciences

**INTERNATIONAL WORKSHOP ON**  
**Surfaces and Interfaces of**  
**Quantum Materials**

**June 03<sup>rd</sup>-04<sup>th</sup>, 2019**  
**Meeting Room 236, Building M, IOP, CAS**

**Invited Speakers:**

<b>Ward Plummer</b>	<i>Louisiana State University</i>
<b>Sokrates Pantelides</b>	<i>Vanderbilt University</i>
<b>Jak Chakhalian</b>	<i>Rutgers University</i>
<b>Jiandi Zhang</b>	<i>Louisiana State University</i>
<b>Jianming Zuo</b>	<i>University of Illinois</i>
<b>Tom Wu</b>	<i>University of New South Wales (UNSW), Sydney</i>
<b>Jian Liu</b>	<i>University of Tennessee, Knoxville</i>
<b>Felix Trier</b>	<i>Université Paris-Saclay</i>
<b>Jian Shen</b>	<i>Fudan University</i>
<b>Zhigao Sheng</b>	<i>Hefei Institute of Physical Science, CAS</i>
<b>Cheng Song</b>	<i>Tsinghua University</i>
<b>Yuefeng Nie</b>	<i>Nanjing University</i>
<b>Andreas Herklotz</b>	<i>Martin-Luther-University Halle-Wittenberg</i>
<b>Lin Gu</b>	<i>Institute of Physics, CAS</i>
<b>Pu Yu</b>	<i>Tsinghua University</i>
<b>Yanwei Cao</b>	<i>Ningbo Institute of Materials Technology and Engineering, CAS</i>
<b>Anquan Jiang</b>	<i>Fudan University</i>
<b>Tong Zhang</b>	<i>Fudan University</i>
<b>Chungang Duan</b>	<i>East China Normal University</i>
<b>Chen Ge</b>	<i>Institute of Physics, CAS</i>
<b>Meng Meng</b>	<i>Institute of Physics, CAS</i>

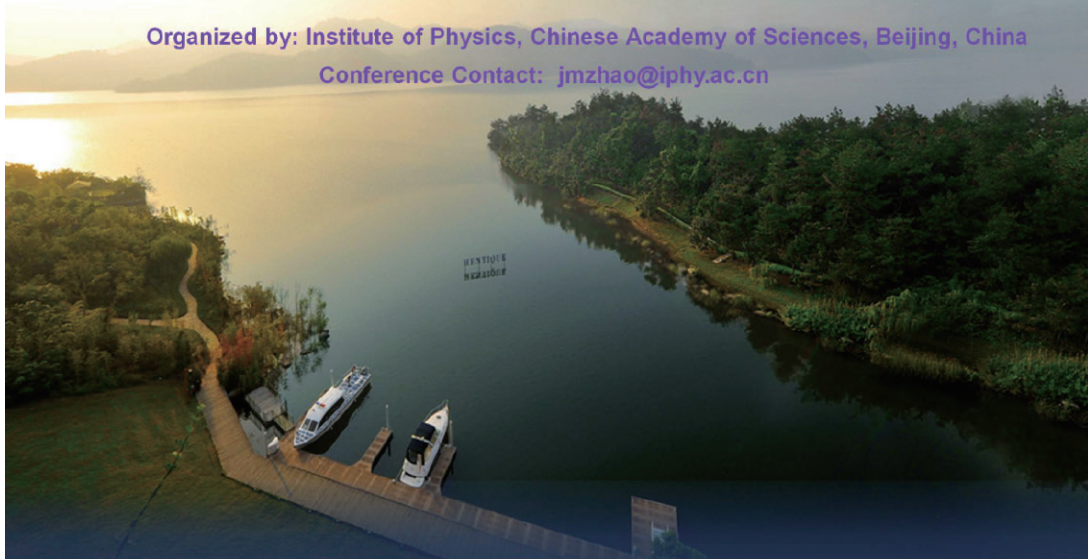
Organizer: State Key Laboratory for Surface Physics, Institute of Physics, CAS  
中国科学院物理研究所表面物理国家重点实验室  
Contact: Ms. QiuHong LI (Email: surface@iphy.ac.cn, 010-82649428)

## 1st International Conference on Ultrafast Spectroscopy of Correlated Quantum Materials (USCQM - 2019)

July 14 - 17, 2019, Liyang, China

Organized by: Institute of Physics, Chinese Academy of Sciences, Beijing, China

Conference Contact: [jmzhao@iphy.ac.cn](mailto:jmzhao@iphy.ac.cn)



The USCQM conference is to boost the international research on ultrafast spectroscopy of quantum materials, with an emphasis on correlated systems and an extension to all various time-resolved ultrafast spectroscopies. The conference aims to provide a platform for international colleagues of the ultrafast spectroscopy community to report their latest results, exchange information and ideas, and foster collaborations.

### Confirmed Invited Speakers (by Surname)

- Prof. Andrea Cavalleri, MPI & Oxford Univ.
- Prof. Jiangping Hu, Inst. of Physics, CAS
- Prof. Roberto Merlin, Univ. of Michigan
- Prof. Dragan Mihailovic
- Prof. Joseph Orenstein, U. C. Berkeley
- Prof. Z. -X. Shen, Stanford Univ.
- Prof. Q. -K. Xue, Tsinghua Univ.
- Prof. Nanlin Wang, Peking Univ.
- Prof. Jimin Zhao, Inst. of Physics, CAS

### Conference Chairs

JiMin Zhao, NanLin Wang

### Important Dates

Registration & abstract submission open: Jan. 1, 2019

On-site registration: July 14, 2019

Conference: July 15-17, 2019

<http://Official website to come up soon>

## 2019-2020 年引进人才介绍

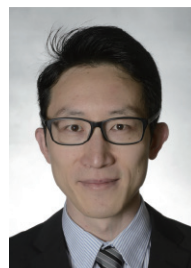
章一奇  
Yiqi Zhang



章一奇，2003年7月毕业于华东理工大学物理系，获得工学学士学位；2008年获得中国科学技术大学聚态物理博士学位；2008年至2011年在德国马克斯普朗克微结构物理研究所开展博士后工作从事金属表面纳米磁结构研究；2011年至2015年在德国慕尼黑工业大学物理系继续博士后工作，开展界面新型分子纳米材料研究，并于2015年晋升为高级研究员；2020年1月加入中国科学院物理研究所，任特聘研究员，博士生导师。目前主要研究方向为利用分子设计结合超高真空环境下界面反应，构筑功能性复杂结构分子晶体 (Nat. Chem. 10, 296, 2018) 以及具有人工结构的二维 $\pi$ 共轭有机分子单层 (Nat. Commun. 3, 1286, 2012; J. Am. Chem. Soc. 141, 5087, 2019)。利用扫描探针显微镜结合光电子能谱等表面表征技术获得分子材料的微观结构 (Angew. Chem. Int. Ed. 56, 7797, 2017) 和电子在材料中的特殊量子态 (Nano Lett. 16, 4274, 2016)。

Yiqi Zhang received his B.S. degree from East China University of Science and Technology in 2003, and PhD degree in condensed matter physics at University of Science and Technology of China in 2008. He conducted postdoctoral researches at Max Planck Institute of Microstructure Physics in the following three years, investigating magnetic surface nanostructures. In 2011, he moved to Technical University of Munich and started new researches in interfacial molecular nanoscience, and was promoted to a senior researcher in 2015. In 2020, he returned to China and became an associated professor at Institute of Physics, Chinese Academy of Sciences. His present researches focus on combining molecular precursor design and on-surface synthesis to construct 2D complex molecular tessellations (Nat. Chem. 10, 296, 2018) as well as  $\pi$ -conjugated molecular networks with novel functionalities (Nat. Commun. 3, 1286, 2012; J. Am. Chem. Soc. 141, 5087, 2019). In particular, scanning probe microscopy and photoelectron spectroscopy are employed to study the pertaining structural (Angew. Chem. Int. Ed. 56, 7797, 2017) and the quantum electronic properties (Nano Lett. 16, 4274, 2016).

## 人才引进及培养



田学增  
Xuezheng Tian

田学增，2009年于山东大学物理学基地班获得学士学位，2014年于物理研究所获得凝聚态物理专业理学博士学位。2014年9月至2016年11月于新加坡国立大学（NUS）和加州大学伯克利分校（UCBerkeley）从事联合博士后项目。2016年12月至2020年9月于加州大学洛杉矶分校（UCLA）从事博士后研究，期间参与三维原子成像（AET）算法的开发。2020年10月加入物理研究所，任特聘研究员，博士生导师。研究领域为电子显微方法学，主要包括：基于电子显微学的多维度成像方法开发，低维量子材料、功能氧化物、非晶态物质等材料的构效关系。田学增参与开发的AET算法可以直接对材料的三维原子坐标直接定位，针对不同材料精度可以达到4-19皮米，应用此方法，他们首次揭示了相变成核的时间分辨三维原子像（Nature, 570, 500-503, 2019），首次研究了掺杂原子的三维局域化效应（Nature Materials, 19, 867-873, 2020），以及首次解析了两种非晶金属的原子结构（Nature, accepted）。

Xuezheng Tian joined the IOP-CAS as an Associate Professor in Oct, 2020. He obtained his Bachelor's degree on Physics from Shandong University in 2009, Doctor's degree on Condensed Matter Physics from IOP-CAS. After graduation, He lead an joint postdoctoral program at NUS and UC Berkeley working on in situ liquid cell electron microscopy. Then, he joined UCLA for another postdoctoral research team, where he is one of the chief member for the development and application of atomic electron tomography (AET) method. His research mainly spans in electron microscopy, including: development and application of new imaging algorithms based on 3D atomic electron tomography and new imaging methodology, towards physics problem in 2D quantum materials, functional oxides, amorphous materials, etc. The AET method Tian co-developed is capable to locate 3D coordinates of atoms in a material with picometer precision, for example, they imaged the 3D atomic nucleation process for the first time (Nature, 570, 500-503, 2019), the 3D localized doping effect in semiconductors (Nature Materials, 19, 867-873, 2020), and deciphered the 3D atomic structure of two amorphous solid for the first time (Nature, accepted).

孟梦  
Meng Meng



孟梦，2017年12月毕业于中山大学，获得理学博士学位；2018一月至今先后以博士后、副研究员身份在中国科学院物理研究所从事科研工作。主要研究方向包括：低维氧化物异质结的可操控外延生长；氧化物异质界面新奇物性与调控；氮化物/氧化物杂化异质结的磁、输运性质。例如：通过构筑BaTiO<sub>3</sub>/SrRuO<sub>3</sub>/BaTiO<sub>3</sub>异质结，首次实现了磁性极化金属相，揭示了复杂氧化物中电子-晶格-自旋之间独特的耦合作用 (Nat. Commun. 10, 1-7 (2019))。成功制备了Mn<sub>4</sub>N/MgO异质结，并对其反常霍尔效应进行了系统的研究，证明了锰氮化合物是开发可持续自旋电子学设备的一个理想材料 (Appl. Phys. Lett. 106, 032407 (2015))，并通过化学掺杂 (Appl. Phys. Lett. 109, 082405 (2016)) 和结构相控制 (Appl. Phys. Lett. 112, 132402 (2018)) 对其自旋输运性能进行调控。

Meng Meng obtained his Ph. D. from Sun Yat-sen University in December 2017. Since Jan. 2018, he has been engaged in scientific research at the Institute of Physics, Chinese Academy of Sciences as a postdoctoral fellow and then as an associate professor. His main research interests include: controllable epitaxial growth of low-dimensional oxide heterostructures using advanced thin-film epitaxial techniques; discovery and control of emergent phenomena at oxide heterointerfaces; Magnetic and transport properties of nitride/oxide heterostructure. For example, by constructing BaTiO<sub>3</sub>/SrRuO<sub>3</sub>/BaTiO<sub>3</sub> heterostructure, a magnetic polar metal phase was realized for the first time, revealing the unique coupling between charge, lattice and spin in complex oxides (Nat. Commun. 10, 1-7 (2019)); Growth of Mn<sub>4</sub>N/MgO heterostructure and systematically studied its anomalous Hall effect, proving that Mn-N compound is a promising candidate for developing sustainable spintronics devices (Appl. Phys. Lett. 106, 032407 (2015)). Furthermore, the spin-based transport properties was controlled by chemical doping (Appl. Phys. Lett. 109, 082405 (2016)) and structural phases (Appl. Phys. Lett. 112, 132402 (2018)).



## 人才引进及培养

王理  
Li Wang



王理，2009年6月毕业于武汉大学物理学院，获得理学学士学位；2016年6月在武汉大学物理学院获得凝聚态物理博士学位，期间曾在美国麻省理工学院和田纳西大学联合培养学习2年；2016年至2020年在中国科学院物理研究所，表面物理国家重点实验室从事博士后研究；2020年12月留所，任副研究员。主要研究方向包括：大尺寸二维单晶生长 (Nature 2019, 570, 91)；大尺寸金属单晶生长 (Nature 2020, 581, 406)；二维材料超快生长 (Nat. Chem. 2019, 11, 730) 等。

Li Wang obtained B. S. Degree in June 2009 and Ph. D. Condensed Matter Physics in June 2016 from School of Physics and Technology, Wuhan University. During this period, he was the Joint student at Massachusetts Institute of Technology and University of Tennessee at Knoxville for 2 years. He was the postdoctoral researcher from 2016 to 2020 and became associate professor since December 2020 at the State Key Laboratory of Surface Physics at the Institute of Physics, Chinese Academy of Sciences. Now his research interests are large-scale two-dimensional single crystal growth (Nature 2019, 570, 91); large-scale metal single crystal growth (Nature 2020, 581, 406); ultra-fast growth of two-dimensional materials (Nat. Chem. 2019, 11, 730), etc.

李晓敏  
Xiaomin Li



李晓敏 2011-2017 年就读于中科院物理所取得凝聚态物理博士学位。博士期间主要工作是利用原位透射电镜技术，研究氧化铈中氧空位的产生和修复的动力学过程以及涉及的氧化还原化学过程。相关工作有 Applied Physics Letters. 2015, 107, 211902; ChemCatChem. 2016, 8, 3326-3329. 等。2017 年 -2019 年在北京大学物理学院继续博士后研究。主要工作是参与搭建日本电子 JEM-ARM300F 双球差校正透射电镜及相关探测设备等，以及利用原位球差电镜技术研究氧化铈纳米颗粒加热下的缺陷结构。相关工作有 Sci. China. Chem.2019, 62, 1704-1709. 等。2019 年 9 月以副主任工程师身份入职中科院物理所，主要研究方向为：球差电镜技术及其科研应用；原位电镜技术应用研究。

Xiaomin Li got her Ph.D. in physics with honor from Institute of Physics Chinese Academy of Sciences, China in 2017. From 2017 to 2019 she joined School of Physics, Peking University as postdoctoral appointee mainly working on in situ aberration-corrected transmission electron microscopy. Since Sep. 2019, she joined the State Key Laboratory for Surface Physics as an senior engineer. Her research interests mainly focus on aberration-corrected transmission electron microscopy technique and its scientific application; in situ transmission electron microscopy technique.

# H 荣誉和奖励 onors and Awards

## 获奖情况

### 职工获奖情况

姓名	所获荣誉
郭建东	中国物理学会胡刚复奖 (2019)
吴克辉、陈岚、冯宝杰、程鹏、孟胜	北京市科学技术奖自然科学奖一等奖 (2019)
鲁年鹏	J.Phys.: Conden. Matter (JPCM) 期刊评选的 “Emerging Leaders 2020”
孟 胜	国家自然科学基金委杰出青年 (2020)
孟 胜	优秀科研实践指导教师 (2020)

### 研究生获奖情况

#### ◆中国科学院大学 2018-2019 学年优秀学生

三好学生: 李晓梅 王建林 余博晗 纪桂萍 赵新佳 加孜拉·哈赛恩 苗光耀 徐小凤 安齐昌 朱 清  
李淑荟 张 平 徐纪玉 关梦雪 张 进  
优秀毕业生: 孙丽欢

#### ◆中国科学院物理研究所 2019 年度所长奖学金优秀奖

陈彩云 关梦雪 李晓梅 赵新佳 苗光耀 孟利楠

#### ◆中国科学院物理研究所 2019 年度所长奖学金表彰奖

朱 亮 王建林 郭金键 余博晗 唐向前 陈晓钰 加孜拉·哈赛恩 林子荐 王珍珍 李淑荟 张 平  
张和煦 张嘉翔 胡史奇 申钰田 游佩桅 李轩熠

#### ◆ 2019 年研究生国家奖学金 徐纪玉 (博士) 陈 潘 (博士)

#### ◆中国科学院大学 2019-2020 学年优秀学生

三好标兵: 王建林  
三好学生: 郭金键 孙华聪 刘欣宇 陈笑坤 唐向前 安 旻 陈晓钰 薛思玮 安齐昌 林子荐 胡文启  
张和煦 李文辉 胡史奇 游佩桅 张圣杰 李轩熠  
优秀毕业生: 朱 亮

#### ◆中国科学院物理研究所 2020 年度所长奖学金优秀奖

蔡 尘 陈晓钰 薛思玮 张圣杰 岳绍圣 胡史奇

#### ◆中国科学院物理研究所 2020 年度所长奖学金表彰奖

张晓伟 廖 磊 孙华聪 陈笑坤 安 旻 唐向前 田珍耘 安齐昌 徐小凤 苗光耀 李文辉 耿岱玉  
刘慧如 刘新豹 宋晨晨 贾华显 周 辉 陈大强 张一民

#### ◆ 2020 年研究生国家奖学金 余博晗 (博士) 王 宇 (博士) 赵儒翼 (硕士)

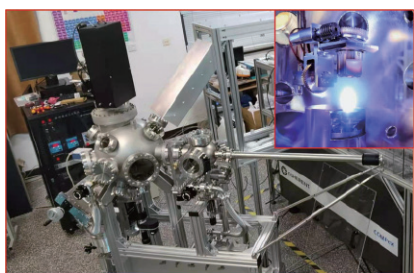
## 特色仪器



### 双球差校正透射电子显微镜

型号：JEM-ARM300F。功能：材料原子像、元素分析与谱成像，性能：STEM 分辨率：63 pm@300 kV，TEM 分辨率：80 pm@300 kV，EELS 能量分辨率：0.35 eV，EDS 能量分辨率：133 eV。

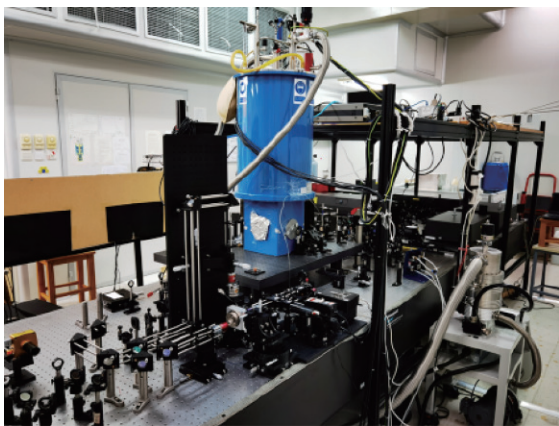
Model: JEM-ARM300F. Function: structure and composition characterization at atomic level. Performance: STEM resolution is 63 pm@300 kV, TEM resolution is 80 pm@300 kV. EELS energy resolution is 0.35 eV, and EDS energy resolution is 133 eV.



### 脉冲激光沉积系统 (Pulsed Laser Deposition-PLD)

对于脉冲激光沉积方法 (PLD)，在较高生长温度下，沉积原子在面内方向具有较大的扩散平均自由程，其生长过程非常接近热力学平衡状态，可以得到很高结晶质量的氧化物外延单晶薄膜。此外，配合高能电子束衍射技术 (RHEED)，还可以实现以原胞甚至单原子层为单元的生长过程精确控制，所以 PLD 方法也可以进行具有单原子层分辨的氧化物异质结或超晶格的构建。

For the pulsed laser deposition (PLD) method, the deposited atoms can move laterally on the surface due to the high growth temperature that the growth condition is very close to the thermodynamic equilibrium state, from which we can obtain high quality crystal oxide epitaxy thin films. Furthermore, under the assistance of reflection high energy electron diffraction (RHEED), we can monitor the growth process at the atomic level of unit cell or crystal lattice, and then realize the fabrication of oxide heterojunctions and superlattices.



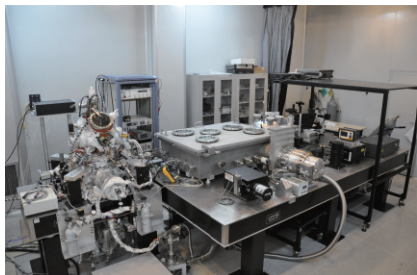
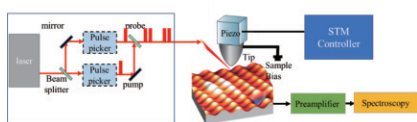
### 在线原位 (on-site in situ) 高压泵浦 - 探测超快光谱实验装置

(On-site in situ high pressure pump-probe ultrafast spectroscopy instrument)

超快光谱学 and 高压物理学以往是两个独立的凝聚态物理学科，如果将二者结合起来，不仅实现仪器研发的突破和进步，而且发现压强诱导的超快动力学特性，将有望开启和促进一个新的“高压超快科学”交叉领域，对促进极端条件下的凝聚态物理研究有重要意义。赵继民与合作者成功搭建了一套在线原位 (on-site in situ) 的高压泵浦 - 探测超快光谱实验装置，该实验装置采用背

散射校压和气膜加压等技术并有机地集成，能够保证在调压校压过程中样品和 DAC 都保持不移动不旋转不被拿出光路，从而避免引入人为误差，提高了数据的可靠性。传统“原位”实验仅要求样品不拿出 DAC，而“在线”实验进一步要求 DAC 和样品都固定在光路里，以前鲜有报道，在线原位实验对双光路精准实验尤为重要。赵继民等利用这个装置研究了强关联材料  $\text{Sr}_2\text{IrO}_4$  的高压超快动力学，发现了压强诱导的声子瓶颈效应，增添了新的凝聚态物理知识。该套装置目前可实现压强调节范围在 0–44.5 GPa 甚至更高，时间分辨率达到 50 fs 甚至更小。

Ultrafast spectroscopy and high pressure physics are conventionally two isolated independent research areas. If we integrate them together by not only instrumentation innovations but also discovering high pressure induced ultrafast dynamics properties, then we are able to initiate a new cross area “high pressure ultrafast science”, which is essential to the investigation of condensed matter physics under extreme conditions. Recently Prof. Jimin Zhao et al. successfully constructed an on-site in situ high pressure pump-probe ultrafast spectroscopy instrument. By integrating back-scattering and gas membrane techniques coherently, they achieved such that both the sample and the DACs are fix during the experiment, without any motion, rotation, or taking-out of the light path, including the tuning and calibrating pressure procedures. This avoided introducing artifacts, thus assuring reliable data. Conventional in situ experiments means the sample is not taking out of the DACs. Here on-site experiment means that both the sample and the DACs are not taken out of the light path. The on-site in situ experiment is crucial for two beam experiments, such as the pump-probe experiments. With this innovated instrument, Zhao et al. investigated the ultrafast dynamics of strongly correlated  $\text{Sr}_2\text{IrO}_4$ , whereby they discovered pressure-induced phonon bottleneck effect—a new knowledge to condensed matter physics. Currently the instrument functions with a pressure tuning range coving at least 0–44.5 GPa and a temporal resolution limited only by conventional pump-probe experiments, that is at least 50 fs.



## 超快激光耦合扫描隧道显微镜系统 (Photo STM)

该系统结合超高真空 STM 的原位空间分辨和超快激光的泵浦探测技术，在传统的扫描隧道显微镜的基础上，实现了隧道电子谱的时域激发和探测，并获得了飞秒 / 皮秒 / 纳秒时间分辨的 STM 原位探测功能。具体特性包括：

- 兼容了光学激发及探测的扫描探针 STM 扫描头，兼顾了低温稳定性和超高真空系统，在保持原子级空间分辨率的基础上实现了隧穿电流 / 隧道电子谱的时域测量，并兼容了电学 / 光学激发 - 原位光谱的测量；
- 超高真空系统的激光定位耦合装置，可实现激光光斑在针尖 - 样品结的定位和长时间稳定；
- 激发波长可以覆盖深紫外 (175-185nm) - 蓝光 (350-370nm)- 近红外波段 (700-1000nm)；
- 超快时间分辨泵浦探测系统的工作范围能覆盖从飞秒，到皮秒、纳秒，以至亚微秒范围的隧道电子谱的时间演变测量；
- 样品表面处理，分子原位蒸镀。



## 能量 / 动量二维解析的高分辨电子能量损失谱仪 (High-resolution electron energy loss spectroscopy with 2D energy-momentum mapping)

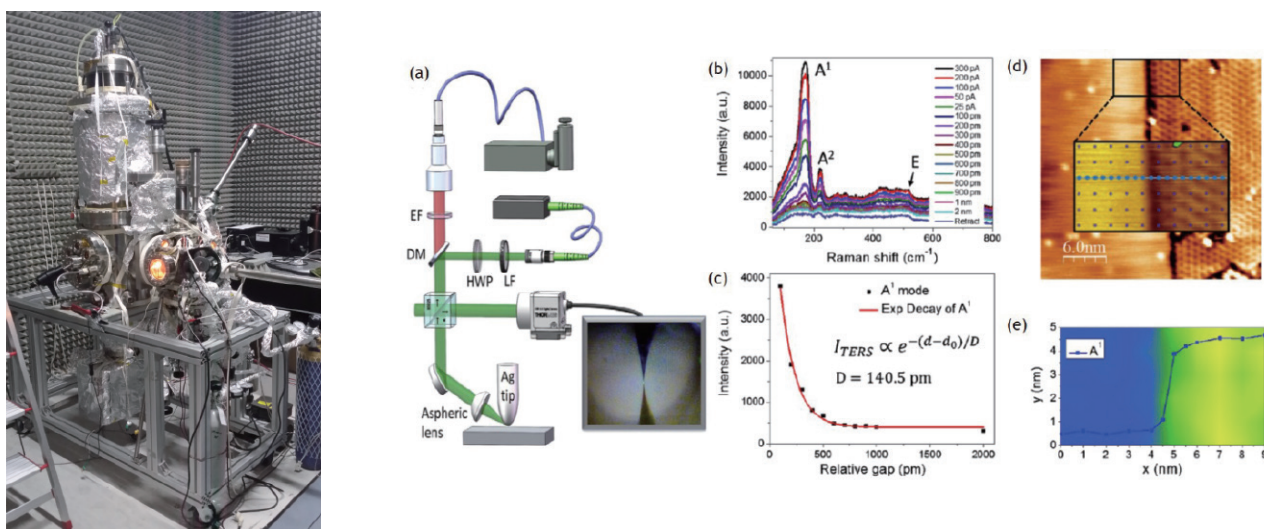
该谱仪使用半球形电子能量分析器与多通道板电子倍增探测器实现对电子信号的二维高效探测，在保证高分辨率的前提下可将动量分辨测量的效率提高一个数量级；在不延长测量时间的前提下将动量空间的采样密度提高三个数量级，更好地发挥出谱仪高分辨率的优势；而且具备和角分辨光电子能谱仪的兼容性，可以同时给出电子能带与声子等准粒子分布的本征数据。其超高真空系统的本底压强达到  $3 \times 10^{-10}$  mbar；分析室具有双层金属屏蔽，内部剩余磁场小于 2 mG；样品台具备三维平动、三维转动调节自由度，同时具有液氮到室温的控温功能；谱仪激发电子束的能量线宽好于 0.67 meV，角度分布小于  $0.08^\circ$ ，保证了设计指标的实现，即能量分辨率好于 1 meV，动量（角度）分辨率好于  $0.8^\circ$ 。

The energy/momentum two-dimensionally resolved HREELS (2D-HREELS) employs the hemispherical electron energy analyzer and the multiple channel plate (MCP) to detect the 2D electron signals efficiently and sensitively. Therefore it possesses higher efficiency of momentum-resolved measurements by an order of magnitude than conventional spectrometers without deteriorating the resolution of energy or momentum. Also it enhances the density of sampling points in momentum space by three orders

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of magnitudes than conventional spectrometers without extending the measurement time. Additionally, the 2D-HREELS is totally compatible with angle-resolved photoelectron spectroscopy (ARPES), being able to provide the intrinsic data on both electrons and phonons with high precision in E and k space. The base pressure of the ultrahigh vacuum system is  $3 \times 10^{-10}$  mbar; the double-layered metal shield of the analysis chamber ensures the residual magnetic field being lower than 2 mG. The sample stage is attached on a six-dimension manipulator with temperature controlled between liquid helium temperature and room temperature. The energy width of the primary electron beam can be better than 0.67 meV with the spread angle smaller than  $0.08^\circ$ , achieving the energy and momentum resolutions (1 meV and  $0.8^\circ$ , respectively).

### 光学集成 - 低温 (4K) 扫描隧道显微镜 - 针尖增强 Raman 系统 (UHV LT-STM TERS system)



(a) 自主设计的低温 STM-TERS 系统光路示意图。(b) 在硅烯表面测得的不同针尖样品距离下的 TERS 谱，从中可以看出 TERS 对于硅烯的振动模式具有很强的选择性，只有 A1 和 A2 振动峰被极大的增强，而高频处的 E 模式却没有明显增强。通过第一性原理的计算，这种选择性增强效应揭示了单层硅烯的拉曼模式的物理起源。(c) 硅烯的 TERS 光谱表现出随针尖和样品间距离指数的衰减关系。(d) 硅烯的 STM 形貌图。(e) A1 峰的 TERS 强度 mapping 图，从中可以看出其横向空间分辨率可以达到 0.5nm。

拉曼 (Raman) 光谱作为一种重要的原位非破坏性探测技术，能获取分子或者低维材料的特征性振动“指纹”，从而深入表征生物、化学、低维材料等体系的成分和结构，鉴定动力学过程的结构变化。但是传统的拉曼光谱由于散射截面非常小，需要大量的样品才能产生有效信号。因此过去二三十年来，人们又发展了表面增强拉曼 (SERS)、共振拉曼等技术来提高拉曼信号的灵敏度。近年来发展起来的 STM 针尖增强 Raman 技术，通过使用扫描隧道显微镜 (STM) 针尖对电磁场的增

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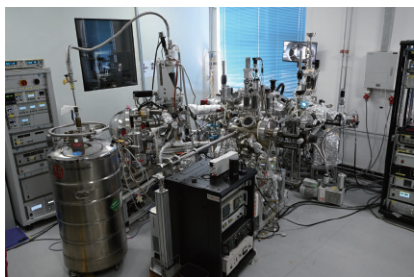
地址：北京市海淀区中关村南三街8号 北京603信箱19分箱  
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强作用发展出针尖增强 Raman 谱 (TERS), 结合 STM 本身所具有的原子分辨及针尖电场对拉曼信号的极大增强, 能够获得单个分子甚至亚分子的拉曼图像, 极大地增强了拉曼光谱的能力, 使得拉曼技术有望在单分子、纳米科学等领域发挥更加突出的作用。

本系统是我们完全自行设计研制的大型系统, 于 2015 年建成并调试成功, 基本功能是在我们的低温 STM 中置入可以三维移动聚焦的透镜组, 将光谱系统和 STM 结合起来, 实现多种工作模式, 例如研究 STM 隧道结的发光、表面结构在光照下的动力学过程、以及 STM 针尖增强 Raman 谱。

Tip-enhanced Raman spectroscopy (TERS), which combined with the scanning probe microscopy (SPM) and Raman spectroscopy, processes the spatial resolution and the capability to access chemical information with ultrahigh sensitivity. It is a powerful tool to study the photon, phonon, electron, plasmon and their interactions, to characterize the nanostructures and nanoptical properties at atomic scale. Based on a home-build low-temperature scanning tunneling microscopy (STM) and MBE union system, we develop the high performance LT-UHV-TERS system. A signal enhancement factor as high as 109 and a TERS spatial resolution of 0.5 nm have been achieved by using silicene on Ag(111) as a prototypical system.



### 角分辨光电子能谱仪 - 扫描隧道显微镜 - 多终端分子束外延生长联合系统 (ARPES-STIM-MBE system)

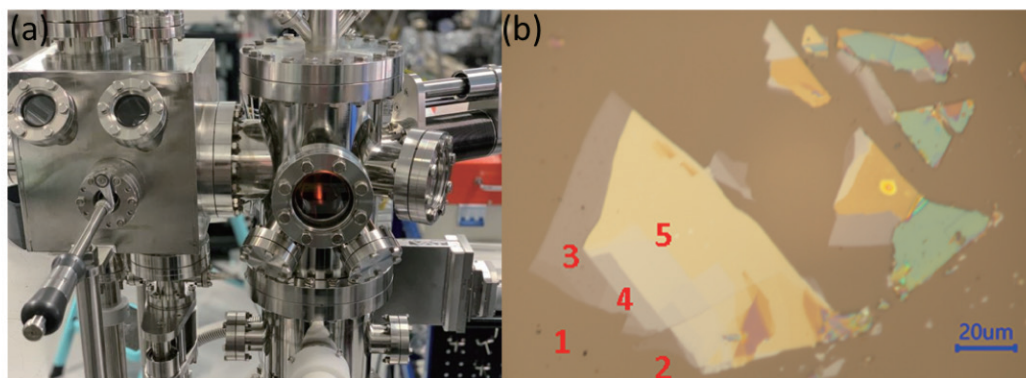
该设备由一套 2018 年购置于 SPECS 公司的 ARPES 系统、自制 MBE 系统以及自制 STM 组成, 各部分通过 UFO 进行真空互联。该系统可以实现新型二维材料的精确制备以及原子结构和电子结构的原位表征。该系统还可以与我们自主研发设计的超高真空原位剥离 - 堆垛系统连接, 进一步拓展研究对象, 探索在这些低维材料中的拓扑、磁性和超导等物性及量子效应。另外, 高次谐波光源正在研

制中, 与 ARPES 结合后可用于探测低维及拓扑量子材料的超快动力学性质。

The system is composed of a commercial ARPES (SPECS), homemade MBE, and homemade STM. Different parts of the system are connected by an UFO chamber which enable the transfer of samples in ultra-high vacuum. Using this system, we can prepare novel 2D materials and investigate their structures and electronic properties in situ. This system can also connect to our homemade "ultrahigh vacuum mechanical exfoliation and stacking system" and make it possible to investigate the topological, magnetic, and superconducting properties in low-dimensional materials. On the other hand, we are developing a high-harmonic generation light source for ARPES, which can be used to investigate the ultrafast dynamic of low-dimensional and topological materials.

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### 新型二维材料的超高真空 (UHV) 原位剥离 - 堆垛系统 (UHV mechanical exfoliation and stacking system)



(a) 自主设计开发的超高真空 (UHV) 原位剥离 - 堆垛系统。(b) 利用该系统解理的少层样品。

自从石墨烯被发现以来，机械解理技术已经成为制备高质量二维材料的重要方法之一。另外，通过解理之后的堆垛技术可以进一步实现二维异质结材料以及转角石墨烯等人造晶体的构筑，实现单一材料无法实现的奇特物性。然而已有的剥离 - 堆垛技术一般是在大气或者手套箱内实现的。将该技术移植到超高真空环境中，可以避免二维材料在大气中被氧化或污染，更利于对其原子结构和电子结构进行原位表征。

依靠我们多年的超高真空系统的设计与使用经验，我们成功地开发了一套超高真空 (UHV) 原位剥离 - 堆垛系统。目前该系统已经实现了超高真空下多种层状材料的大面积解理与转移，大大拓展了二维材料及异质结构的种类，为下一步 STM 和 ARPES 研究打下了基础。

Since the discovery of graphene, mechanical exfoliation has become one of the most important techniques for fabricating 2D materials. In addition, stacking of different materials can realize novel artificial crystals, such as 2D heterostructures and twist-angle graphene, which may host unique properties. However, conventional mechanical exfoliation is realized in ambient condition or glove box. Realization of mechanical exfoliation in ultrahigh vacuum can prevent the contamination of 2D materials and facilitate the investigation of their structures and electronic properties.

Recently, we developed an ultrahigh vacuum mechanical exfoliation and stacking system. We have realized the exfoliation and transfer of various 2D materials in ultrahigh vacuum condition. This technique greatly enriches the variety of 2D materials and heterostructures that can be investigated by surface-sensitive techniques, such as STM and ARPES.