中国科学技术大学
University of Science and Technology of China

2018 EXCITED

1st Workshop on Excited States in Condensed Matter Physics

June 9 – 10, 2018
Hefei, China

Sponsored by

National Natural Science Foundation of China

International Center for Quantum Design of Functional Materials

Key Laboratory of Strongly–Coupled Quantum Matter Physics

Workshop Manual

Mission of the Workshop

The 1st Workshop on Excited States in Condensed Matter Physics aims to provide a platform for experimental and theoretical physicists working on the excited state dynamics in condensed matter systems to share their recent developments in frontiers of experiment and theory.

In addition to the lectures given by the invited speakers, a half-day training session on a time-dependent *ab initio* non-adiabatic molecular dynamics package (Hefei-NAMD) will be delivered. Hefei-NAMD is an *ab initio* nonadiabatic molecular dynamics program to investigate the ultrafast excited carrier dynamics in real and momentum space, energy and time scale.

This workshop will be mainly supported by the fund from the National Natural Science Foundation of China, the International Center for Quantum Design of Functional Materials (ICQD) at USTC and the Key Laboratory of Strongly-Coupled Quantum Matter Physics.

Invited Speakers

- Jun Cheng (程俊), Xiamen University
- Zhixin Hu (胡智鑫), Tianjin University
- Hong Jiang (蒋鸿), Peking University
- Minbiao Ji (季敏标), Fudan University
- Wei Ji (季威), Renmin University
- Kaihui Liu (刘开辉), Peking University
- Xinzheng Li (李新征), Peking University
- Sheng Meng (孟胜), Institute of Physics, Chinese Academy of Sciences
- Yuchen Ma (马玉臣), Shandong University
- Shijing Tan (谭世倞), University of Sciences & Technology of China
- Fengqiu Wang (王枫秋), Nanjing University
- Rui Wang (王瑞), National Center for Nanoscience and Technology
- Yihua Wang (王熠华), Fudan University
- Yao Yao (姚尧), South China University of Technology
- Bingbing Zhang (张兵兵), Institute of High Energy Physics
- Chunfeng Zhang (张春峰), Nanjing University
- Haiming Zhu (朱海明), Zhejiang University
- Jin Zhao (赵瑾), University of Sciences & Technology of China
- Qun Zhang (张群), University of Sciences & Technology of China
- Shengbai Zhang (张绳百), Rensselaer Polytechnic Institute

Program of the Workshop

Venue: Exhibition Hall in the Hefei National Laboratory Building, USTC

(地点：合肥微尺度物质科学国家研究中心一楼科技展厅)

Saturday, June 9		
Session 1 Chair: 赵瑾		
09:00 - 09:10	**Opening Remarks**	
09:10 - 09:45	Shengbai Zhang (张绳百)	Recent Development in Phase Change Memory Materials using Time-dependent Density Functional Theory
09:45 - 10:20	Minbiao Ji (季敏标)	Imaging 2D Materials with Pump-Probe Microscopy
Coffee Break & Group Photo		
Session 2 Chair: 蒋鸿		
10:40 - 11:15	Jun Cheng (程俊)	Level Alignment Across Electrochemical Interfaces
11:15 - 11:50	Qun Zhang (张群)	Probing Photoexcited Hole Dynamics in Photocatalytic Nanomaterial Systems by Ultrafast Spectroscopy
Lunch Time		
Session 3 Chair: 李新征		
13:30 - 14:05	Hong Jiang (蒋鸿)	Numerically Accurate *GW* Approach to Electronic Band Structure of Materials
14:05 - 14:40	Fengqiu Wang (王枫秋)	低维材料光电物性调控及器件应用
14:40 - 15:15	Wei Ji (季威)	非平衡态下的几何结构弛豫和电子诱导反应模拟
15:15 - 15:30	Bingbing Zhang (张兵兵)	多尺度超快 **X** 射线衍射方法发展及应用
Coffee Break		

Session 4 Chair: 王枫秋		
15:50 - 16:25	Chunfeng Zhang (张春峰)	Ultrafast Coherent Effects in Organic Solar Cells
16:25 - 16:50	Yao Yao (姚尧)	Simulation of Ultrafast Exciton Dynamics in Organic Materials
16:50 - 17:25	Jin Zhao (赵瑾)	Dynamics of Excited Carriers Investigated by Non-Adiabatic Molecular Dynamics
17:25 - 17:40	Zhixin Hu (胡智鑫)	金属表面电诱导反应的分子动力学研究
Dinner Time		
Sunday, June 10		
Session 5 Chair: 谭世俍		
09:00 - 09:35	Kaihui Liu (刘开辉)	Ultrafast Optical Spectroscopy of Individual Nano-materials with Defined Atomic Structure
09:35 - 10:10	Sheng Meng (孟胜)	Photoexcited Dynamics and Emergence of New States in Two-dimensional Materials
Coffee Break		
Session 6 Chair: 孟胜		
10:30 - 11:05	Yihua Wang (王熠华)	Light-matter Interaction in Quantum Materials
11:05 - 11:40	Yuchen Ma (马玉臣)	生物体系和半导体缺陷激发态的多体格林函数理论研究
11:40 - 11:55	Rui Wang (王瑞)	二维层状材料的超快光谱研究
Lunch Time		
Session 7 Chair: 刘开辉		
13:30 - 14:05	XinZheng Li (李新征)	凝聚态体系中一些由核量子效应诱发的新物性

14:05 - 14:40	Haiming Zhu (朱海明)	Photoexcitation Dynamics at 2D van der Waals Interface
14:40 - 15:15	Shijing Tan (谭世倞)	金属半导体界面等离激元增强的热电子过程
15:15 – 15:25	**Closing Remarks**	
15:30 - 17:30	**Training Session (理化大楼 9004)**	

Abstracts of Invited Talks

Recent Development in Phase Change Memory Materials using Time-dependent Density Functional Theory

Shengbai Zhang

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Phase change memory (PCM) materials exhibit fascinating physics as SET (i.e., its amorphiszation) happens in less than a 100 fs, while RESET (i.e., its recrystallization) happens in a matter of only a few ns, which defies exclusively all the phase-change phenomena known for solid state. They are the backbone of DVD, as well as that of electronic memory devices such as IBM's storage class memory and the recent Micron's X-Point technology. Most recently, PCM also gained momentum for developing non-von Neumann architecture, beyond CMOS, and in-memory computing. Our journey on the quest of the PCM materials started with the understanding of phase transitions using static [1] and quasi-static [2] first-principles calculations. Nonetheless, a non-thermal nature of the ultrafast PCM material amorphization under a high electronic excitation was unveiled for the first time [2], which has since gained considerable momentum. Using the recently developed time-dependent density functional theory (TDDFT)-molecular dynamics (MD), we not only confirmed the previous predictions, but also uncovered the dependence on the excitation energies – a high enough excitation energy inevitably leads to a significant carrier multiplication effect [3]. As such, a phase transition takes place well before the lattice can be heated up. A similar phenomenon found in standard semiconductors, coined with the name plasma quenching, was also explained by our theory [4]. Most recently, we found that, in ferroelectric materials, an equally ultrafast (< a few 100's fs) phases transition can take place *between crystalline phases*. While this proposition is in startle contrast to our naïve intuition, it is in full agreement with experiments [5].

Work in collaboration with X.-B. Li, X.Q. Liu, X. Han, J. Bang, S. Meng, and companies.

[1] X. Q. Liu, et al., Phys. Rev. Lett. **106**, 025501 (2011).
[2] X.-B. Li, et al., Phys. Rev. Lett. **107**, 015501 (2011).
[3] J. Bang, Y. Y. Sun, X.-Q. Liu, F. Gao, and S. B. Zhang, Phys. Rev. Lett. **117**, 126402 (2016).
[4] C Lian, SB Zhang, S Meng, Phys. Rev. B **94**, 184310 (2016).
[5] N.-K. Chen, et al., Phys. Rev. Lett. **120**, 185701 (2018).

Imaging 2D Materials with Pump-Probe Microscopy

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Abstract:
Pump-probe microscopy measures the ultrafast transient optical properties of materials with decent spatial and temporal resolution. In this talk, I will introduce our recent work on studying the carrier and coherent phonon dynamics in few-layer black phosphorus with strong layer-dependence. I will also discuss our preliminary results on the transient behaviors of twisted bilayer graphene, especially at the Van Hove singularity.

Background:
Dr. Minbiao Ji received B.S. degree in Physics from the Peking University, Beijing, in 2001. He received his Ph.D degree in Physics at Stanford University, in 2011. His research was focused on using ultrafast laser spectroscopy to study various chemical dynamics, including hydrogen-bond dynamics in water, and transient dynamics of carriers and enzyme molecules. Afterwards, he joined the research group of Prof. Sunney Xie at Harvard University as a postdoctoral research fellow, where he learnt the technique of coherent Raman scattering microscopy and applied it to various biomedical researches. Minbiao Ji is currently a Professor in the Department of Physics in Fudan University, Shanghai, where he won the "Thousand Youth Talent Plan" in 2015. His current research is focused on developing novel nonlinear optical spectroscopy and microscopy tools to study biomedical and material sciences.

Level Alignment Across Electrochemical Interfaces

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Electrochemistry is an old branch of science, and the renewed interest is largely due to its important relevance to the contemporary challenges on energy and environment. This offers a good opportunity for theoretical development of this interesting and challenging field. I will first present a density functional theory based molecular dynamics (DFTMD) method for calculation of redox potentials and pKa's, and its application to electrochemical interfaces for computing level alignment and surface acidities. In particular, I will explain a computational standard hydrogen electrode (cSHE) method to align all computed energy levels across electrochemical interfaces to a common reference so that they can be directly compared against experiment. The level alignment will be shown not only to be useful in revealing the negative effect of the shortcomings in density functionals on the electronic energy levels, but also very instructive for understanding electron/proton transfer at electrochemical interfaces. Taking photocatalysis on aqueous TiO2 as an example system, I will show the level alignment of trapped holes near the interface, helping resolve the conflicting interpretations of experimental observations. Furthermore, I will present a novel diagram unifying electronic and protonic energy levels to visualize the thermodynamics of proton coupled electron transfer, providing valuable insight into the thermodynamic overpotentials of water oxidation on TiO2.

[1] J. Cheng*, X.-D. Liu, J. VandeVondele, M. Sulpizi, M. Sprik*, Acc. Chem. Res. 2014, 47, 3522.
[2] J. Cheng*, X.-D. Liu, J. A. Kattirtzi, J. VandeVondele, M. Sprik, Angew. Chem. Int. Ed. 2014, 53, 12046.
[3] J. Cheng*, Joost VandeVondele*, Phys. Rev. Lett. 2016, 116, 086402.
[4] J. Le, M. Iannuzzi, A. Cuesta, J. Cheng*, Phys. Rev. Lett. 2017, 119, 016801.

Probing Photoexcited Hole Dynamics in Photocatalytic Nanomaterial Systems by Ultrafast Spectroscopy

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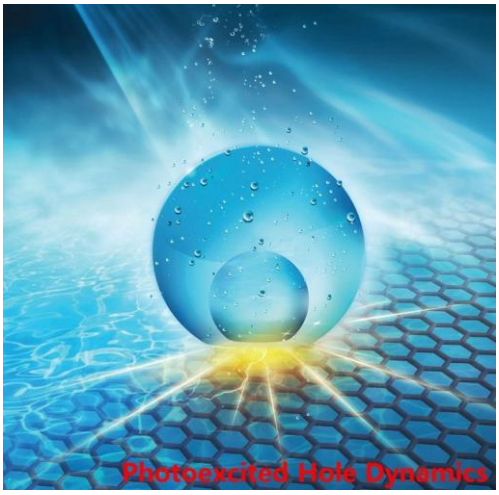
Abstract

In this talk I will report our recent progress in the experimental investigations of photoexcited hole dynamics in photocatalytic nanomaterial systems by means of ultrafast transient absorption spectroscopy. First, we revealed the photoexcited hole transfer in a unique semiconductor–metal–graphene stack structure, which allows for efficiently harnessing charge flow for photocatalysis [1]. Second, we demonstrated a molecular co-catalysis strategy to accelerate hole transfer for enhanced photocatalytic hydrogen evolution [2]. Third, we identified the ultrafast reverse hole transfer at the interface of photoexcited methanol/g-C_3N_4 system, deciphering from the ultrafast hole dynamics perspective the fundamental reason why methanol functions as an efficient hole scavenger in realistic photocatalytic applications [3].



[1] S. Bai *et al*., Adv. Mater. **26**, 5689 (2014).
[2] W. Bi *et al*., Nat. Commun. **6**, 8647 (2015).
[3] Z. Chen *et al*., Angew. Chem. Int. Ed. **57**, 5320 (2018).

Numerically Accurate GW Approach to Electronic Band Structure of Materials

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Many-body perturbation theory in the *GW* approximation is currently regarded as the most accurate and robust first-principles approach to determine electronic band structure of weakly correlated insulating materials without any empirical input. Recent systematic studies of ZnO by several groups clearly indicate the importance of numerical accuracy in the practical implementation of the GW methods. In this talk I will address the challenges for numerically accurate GW calculation based on our recent systematic investigation of the effects of including high-energy local orbitals (HLOs) in the linearized augmented plane waves (LAPW)-based *GW* calculations [1-3]. It is shown that both the accuracy of unoccupied states and the completeness in the summation over states are crucial for numerically accurate *GW* calculations. In general, using LAPW+HLOs basis can significantly improve the performances of the semi-local density functional approximation based GW_0 approach [2]. We have further investigated other systems with electronic configurations that are significantly different from those of common *sp* semiconductors, including VII-IB compounds (MX with M=Cu, Ag and X=Cl, Br and I), transition metal compounds (NiO and FeS_2), and lanthanide oxides (CeO_2 and Ce_2O_3) [3]. We found that the consideration of HLOs in the *GW* based on density-functional theory plus the Hubbard *U* correction (*GW*@DFT+*U*) approach can significantly improve the description of electronic band structure of those d- and f-electron systems.

[1] H. Jiang, R. I. Gomez-Abal *et al.* Computer Phys. Commun.,184, 348(2013).
[2] H. Jiang and P. Blaha, Phys. Rev. B, 93,115203(2016).
[3] H. Jiang, submitted to Phys. Rev. B (2018).

低维材料光电物性调控及器件应用

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王枫秋，男，本科毕业于北京大学电子学系，2009 年获英国剑桥大学电子工程专业博士学位。现任南京大学电子科学与工程学院教授、博士生导师，先后获得国家“青年千人计划”，江苏省“杰出青年科学基金”资助。多年来围绕低维材料光学性质调控、新颖光电器件、以及高性能脉冲激光器等方向开展了多项原创工作。至今在包括 Nature Nanotechnology, Nature Communications, Advanced Materials, ACS NANO 等刊物发表论文 80 余篇。总引用逾 4600 次，其中 10 篇论文引用过百（H 因子=24）。担任国家重点研发计划课题负责人，主持国家自然科学基金面上项目 2 项，参与“量子调控”国家重大科学研究计划项目 1 项，国家重大科研仪器研制项目 1 项，以及澳大利亚 ARC Discovery 项目 1 项。2010 年获得英国皇家工程院 ERA Foundation Award 银奖，并先后入选江苏省“双创人才计划”和江苏省“双创团队计划”。担任激光和光电子领域国际顶级会议 CLEO2016-2018，CLEO2015（亚太）的程序委员会委员。是国际知名综合性学术期刊 *Scientific Reports* 的编委会成员。在国际主流学术会议做邀请报告十余次，是 Nature Communications, ACS Nano 等学术期刊的审稿人。

非平衡稳态下的几何结构弛豫和电子诱导反应模拟

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报告从介绍一种用于模拟 XPS 实验的离子赝势出发，讨论在芯电子受激的非平衡稳态下 PTCDA 分子和 $CuPcF_{16}$ 在 Ag(111)和 Cu(111)表面上，因价电子电荷转移导致的原子结构弛豫[1]。随后的几个例子表明，该离子赝势方法可以进一步推广，用于模拟电荷掺杂下 Te 少层[2]和噻吩/Cu 表面[3]的结构变化和 CrS_2 单、双层的磁性调控[4]，以及探索电子诱导反应的不同反应路径[5-7]。

[1] W. Ji *et al*. Phys. Rev. Lett. **97**, 246101 (2006)
[2] C. Wang *et al*. unpublished (2018)
[3] Z.-X. Hu *et al*. Scientific Reports **4**, 5036 (2014)
[4] C. Wang *et al*. arXiv:1706.10213 (2018) (Phys. Rev. B, in press)
[5] F. Cheng *et al*. ACS NANO **8 (8)**, 8669–8675 (2014)
[6] S.Y. Guo *et al*. J. Phys. Chem. Lett. **6**, 4093–4098 (2015)
[7] F. Cheng *et al*. Chem. Commun. **52**, 6115-6118 (2016)

多尺度超快X射线衍射方法发展及应用

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材料的宏观功能与其微观特性密不可分。除了对平衡态下的各种稳态性质的探索，材料及其在激光作用下所展现出的各种新颖的瞬态特性亦引人入胜。超快X射线衍射技术则将超快激光光谱学和X射线晶体学结合，开创了全新的物理、化学生物等学科交叉的晶格动力学研究领域。随着同步辐射及X射线自由电子激光等大科学装置的发展，超快X射线衍射技术的应用得到极大地拓展。

报告将重点介绍北京同步辐射的两套超快 X 射线探测装置，分别基于实验室的激光打靶等离子体 X 射线光源（~200fs），以及同步辐射装置 1W2B 线站（~150ps）的超快 X 射线衍射装置。以及基于上述平台所开展的低维氧化物超快晶格动力学研究如强关联体系 Sr2IrO4 薄膜、有序化氧空位体系 SrCoO2.5 等。

Ultrafast Coherent Effects in Organic Solar Cells

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In a single-junction solar cell, the power conversion efficiency is limited by the spectrum loss and the excess energy loss. The efficiency was theoretically derived to be less than 33%, known as the Shockley-Quiesser limit. The efficiency limit is further reduced for an organic device due to the loss caused by overcoming the exciton binding energy. In this talk, I'll present our study on the mechanisms of two potential processes to break the limit: singlet exciton fission and coherent charge transfer. Singlet exciton fission can suppress the excess energy loss by converting one photo-excited singlet exciton into two triplets in some organic semiconductors. Coherent charge transfer can avoid the loss during interfacial charge separation due to exciton binding in organic solar cells by employing the effect of quantum vibronic coupling.

Simulation of Ultrafast Exciton Dynamics in Organic Materials

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Benefiting from the recent development of time-resolved spectroscopy technology, people have observed numerous ultrafast excitonic processes in organic materials with the timescale being of tens to hundreds femtoseconds and non-adiabatic phenomena caused by the crossing of potential-energy surfaces. In principle, an accurate solution of the coherent exciton dynamics in molecular systems can help understand these ultrafast non-adiabatic processes, however such kind of molecular dynamics comprising the electron-nuclear couplings is nontrivial and requires breaking the Born-Oppenheimer approximation, which is one of the basic assumptions in quantum chemistry. For the sake of properly dealing with this coherent dynamics, in the recent years several dynamical methodologies have been invoked, but the quantum dynamics simulation for systems with a large number of degrees of freedom is so far a great challenge due to the exponential divergence of the computational cost. In this talk, I present a modified t-DMRG algorithm which can be used to simulate the non-adiabatic processes in realistic molecular system with discrete vibrational modes and vibronic coupling parameters for respective electronic states. I will discuss several cases relating to ultrafast exciton dynamics, such as the charge-transfer process, the singlet fission, and the magneto-electroluminescence in OLED.

Non-Adiabatic Molecular Dynamics Investigations on the Excited Carrier Dynamics

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Abstract

The ultrafast dynamics of photo-excited charge carriers in condensed matter systems plays an important role in optoelectronics and solar energy conversion. Yet it is challenging to understand the multi-dimensional dynamics in time, energy, real and momentum spaces at the atomic scale. Combining the real-time time-dependent Density Functional Theory (TDDFT) with fewest surface hopping scheme, we use homemade time-dependent *ab initio* nonadiabatic molecular dynamics code (Hefei-NAMD) to simulate the excited carrier dynamics in different condensed matter systems including two-dimensional vdW heterostructures and molecule/metal oxide interfaces. The time-dependent dynamics of excited carriers are studied in energy, real and momentum spaces. In addition, the coupling of the excited carriers with phonons, polarons, defects and molecular adsorptions are investigated. Recently, by combining with path-integral techniques, the nuclear quantum effects have been included in the NAMD simulations. Our state of art NAMD studies provide an atomic insight into the ultrafast dynamics of the excited carriers in condensed matter systems.

金属表面电诱导反应的分子动力学研究

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摘要：

金属表面上的分子在外部刺激下可发生成键断键或迁移等变化，理解其中的运动机制将对表面催化和分子机器等领域的研究提供很大帮助[0, 0]。实验中对于表面上单个分子的化学反应同时实现空间和时间分辨是比较困难的。然而理论上却可以通过分子动力学模拟分析整个反应过程中原子运动过程和势能曲线，理解反应机理，预测反应产物。我们以电诱导的表面分子反应作为实例，使用 I2S 模型[0,0]模拟电子激发态，分析原子在电激发后的运动。通过对三个代表性体系研究，我们对表面诱导分子反应中的转动[0]，断键与成键，运动取向的选择等问题有了更深的了解。

关键词：扫描隧道显微镜；分子动力学模拟；表面诱导反应

[1] W.R. Browne, B.L. Feringa, *Nat. Nanotechnol.* **1** (2006) 25–35.
[2] S.P. Fletcher, *Science* **310** (2005) 80–82.
[3] F. Cheng, W. Ji, L. Leung, Z. Ning, J.C. Polanyi, C.G. Wang, *ACS Nano* **8** (2014) 8669–8675.
[4] K. Huang, L. Leung, T. Lim, Z. Ning, J.C. Polanyi, *J. Am. Chem. Soc.* **135** (2013) 6220–6225.
[5] Z. Hu, K. Anggara, J. C. Polanyi, *Chem. Phys. Lett.* **683** (2017) 443-447.

Ultrafast Optical Spectroscopy of Individual Nano-materials with Defined Atomic Structure

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When the characteristic length of a material shrink to 1 nm scale, many distinct physical phenomena, such as quantum confinement, enhanced many-body interactions, strong van der Waals inter-material couplings and ultrafast charge separation, will appear. To investigate the related fascinating low-dimensional physics, we need a tool to quantitatively link the atomic structures to the physical properties of these very small nano-materials. In this talk, I will introduce our recently developed in-situ TEM + high-sensitive ultrafast nanooptics technique, which combines capability of structural characterization in TEM and property characterization in nanooptics on the same individual nano-materials. Several examples of using this technique to study the interlayer quantum coupling and ultrafast dynamics in 1D carbon nanotube system and 2D atomic layered systems will be demonstrated.

[1] Kaihui Liu, Feng Wang* and et al., “High-throughput Optical Imaging and Spectroscopy of Individual Carbon Nanotubes in Devices”, **Nature Nanotechnology 2013**, 8, 917-922.

[2] Kaihui Liu, Enge Wang, Feng Wang* and et al., “Van der Waals-Coupled Electronic States in Incommensurate Double-walled Carbon Nanotubes”, **Nature Physics 2014**, 10, 737-742.

[3] Xu Zhou, Jingxin Cheng, Yubing Zhou, Shiwei Wu*, Hailin Peng*, Kaihui Liu* and et al., “Strong Second-Harmonic Generation in Atomic Layered GaSe”, **JACS 2015**, 137, 7994-7997.

[4] Ziheng Ji, Chuanhong Jin*, Kebin Shi*, Sheng Meng, Kaihui Liu* and et al., "Robust Stacking-Independent Ultrafast Charge Transfer in MoS_2/WS_2 Bilayers", **ACS Nano 2017**, 11, 12020

[5] Jing Liang, Zhipei Sun*, Sheng Meng*, Kaihui Liu* and et al. "Monitoring Local Strain Vector in Atomic-Layered MoSe2 by Second-Harmonic Generation", **Nano Letters 2017**, 17, 7539

[6] Tao Jiang, Hao Hong, Can Liu, Wei-Tao Liu, Kaihui Liu*, and Shiwei Wu*. "Probing Phonon Dynamics in Individual Single-Walled Carbon Nanotubes", **Nano Letters, 2018,** 18, 2590

Photoexcited Dynamics and Emergence of New States in Two-dimensional Materials

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Photoexcitation is a powerful means in distinguishing different interactions and manipulating the states of matter, especially in complex quantum systems. As a well-known charge density wave (CDW) material, 1*T*-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 in 1*T*-TaS_2 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 in TaS_2. In addition, our finding validates nonthermal melting of CDW induced at low light intensities, supporting that conventional hot electron model is inadequate to explain photoinduced dynamics. Our results provide a deep insight on coherent electron and lattice quantum dynamics during the formation and excitation of charge ordering states.

Light-matter Interaction in Quantum Materials

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The coherent interaction between ultrashort light pulses and solid phase of matter have generated a broad spectrum of quantum phenomena ranging from Higgs mode in superconductors to light-induced topological order. I will demonstrate an example where intense far-infrared pulses coherently couple with the surface Dirac fermions of a topological insulator which hybridize into the so-called Floquet-Bloch states. The polarization of the light is a very effective knob to manipulate such a state and can transform the metallic surface into a Chern insulator. I will also propose scanning SQUID as a powerful tool to investigate a zoo of light-induced quantum order.

生物体系和半导体缺陷激发态的多体格林函数理论研究

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多体格林函数理论中的 GW 方法和 Bethe-Salpeter 方程分别可以较高的计算精度研究能带结构和激子性质。我将介绍近几年来课题组利用这两种第一性原理方法尝试解决的几个激发态问题，（1）光合作用体系中类胡萝卜素与叶绿素之间的能量传递[1]，（2）DNA 在水溶液中光吸收的红移[2]，（3）碳纳米管发光的红移[3]，（4）TiO_2 表面缺陷态的来源[4]。

[1] “A new energy transfer channel from carotenoids to chlorophylls in purple bacteria”, Nat. Commun. 8, 71 (2017)
[2] “Charge-transfer excited states in aqueous DNA: Insights from many-body Green function theory”, Phys. Rev. Lett. 112, 228301 (2014)
[3] “Photoluminescence of single-walled carbon nanotubes: The role of Stokes shift and impurity levels”, Phys. Rev. Lett. 111, 137401 (2013)
[4] “Ti Interstitial origin of the band-gap state in TiO_2(110) from GW calculations”, in preparation
[5] “Mediating both valence and conduction bands of TiO_2 by anionic dopants for visible- and infrared-light photocatalysis”, Phys. Chem. Chem. Phys. 20, 12785 (2018)

二维层状材料的超快光谱研究

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维度的减少导致二维层状材料表现出与体材料不同的性质。使用超快光谱技术我们研究了层状材料 α-In_2Se_3 和 1T-TaS_2 体系中载流子的动力学特性。

基于 α-In_2Se_3 薄膜的光电探测器表现出超高的光电响应度。为了探究其机理，参照实际器件，我们研究了 11nm-40nm 厚的 α-In_2Se_3 薄膜在云母及金基底上的动力学性质。发现其在电极处存在非常有效的电荷转移，同时因其载流子寿命、迁移率等其它决定光电流的关键参数与 MoS_2 都是可比拟的，因此我们推测界面电阻以及光电压效应是造成其超高光电响应度的原因。

电荷密度波材料因其与超导材料的相似之处而被广泛关注。1T-TaS2 属于强电声相互体系的派尔斯绝缘体，我们研究了其在不同厚度及不同基底上的相干态声子及其动力学性质，发现其动力学过程包括能量迟豫和单粒子两个过程，厚度对这两个动力学过程均存在很强的调制作用，而且基底直接影响了声子模式的出现。

关键词：α-In_2Se_3, 1T-TaS_2，超高光电响应度，光电压，接触电阻，相干态声子

凝聚态体系中一些由核量子效应诱发的新物性

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有限温度下材料性质的模拟，依据玻恩-奥本海默近似，要求人们对电子结构和原子核的运动分别进行准确的描述。近年来，随着第一性原理电子结构计算方法的发展，电子的量子描述已达到相当的精确度，而与之相应的原子核运动却很大程度停留在经典描述的层次。该处理所带来的一个直接后果是与原子核量子效应相关的诸多物性不能被描述。在该报告中，我们将重点介绍基于第一性原理计算的路径积分的分子动力学方法，用以在实际体系物性模拟中克服类似问题。利用该方法，我们从理论层面研究了核量子效应对氢键系统结构的影响[1-3]、以及高压下轻元素的相图[4-5]。如果时间允许，我们还会对一些与实验组（北京大学江颖研究组）合作完成[6-9]、和纯理论的[10]关于水在固体表面行为研究进行一些的介绍。

关键词：路径积分，分子动力学，核量子效应

[1] X.Z.Li, M.I.J.Probert, A.Alavi, and A.Michaelides, **Phys. Rev. Lett.104**, 066102 (2010) X.Z.Li, B.Walker, and A.Michaelides, **Proc. Nat. Acad. Sci. U.S.A.108**, 6369 (2011)
[2] W. Fang, J. Chen, M. Rossi, Y. X. Feng, X. Z. Li, and A. Michaelides, **J. Phys. Chem. Lett. 7**, 2125 (2016)
[3] J.Chen, X.Z.Li, Q.F.Zhang,M.I.J.Probert, C.J.Pickard, R.J.Needs, A.Michaelides, and E.G.Wang, **Nature Communications 4**,2064(2013)
[4] Y. X. Feng, J. Chen, D. Alfe, X. Z. Li, and E. G. Wang, **J. Chem. Phys. 142**, 064506 (2015)
[5] J.Guo, X. Z. Meng, J. Chen, J. B. Peng, J. M. Sheng, X. Z. Li, L. M. Xu, J. R. Shi, E. G. Wang, and Y. Jiang, **Nature Materials 13**, 184 (2014).
[6] J.Chen, J.Guo, X.Z.Meng, J.B.Peng, J.M.Sheng, L.M.Xu, Y.Jiang, X.Z.Li, and E.G.Wang, **Nature Communications 5**, 4056 (2014)
[7] X. Z. Meng, J. Guo, J. B. Peng, J. Chen, Z. C. Wang, J. R. Shi, X. Z. Li, E. G. Wang, and Y. Jiang, **Nature Physics 11,** 235 (2015)
[8] J. Guo, J. T. Lue, Y. X. Feng, J. Chen, J. B. Peng, Z. R. Lin, X. Z. Meng, Z. C. Wang, X. Z. Li, E. G. Wang, and Y. Jiang, **Science 352**, 321 (2016)
[9] W. Fang, J. O. Richardson, J. Chen, X. Z. Li, and A. Michaelides, **Phys. Rev. Lett. 119**, 126001 (2017)

Photoexcitation Dynamics at 2D van der Waals Interface

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Because of their unique optical and electronic properties, two-dimensional van der Waals heterostructures have shown exciting potential in ultrathin and flexible optoelectronic, valleytronics, photovoltaic and light-emitting devices. As the key steps, the photoexcitation dynamics at van der waals interface determine the overall performance. Despite of a few preliminary studies on this topic, the precise measurements and insights on those processes is still lacking. In this talk, we will apply ultrafast spectroscopy to investigate the photoexcitation dynamics in van der Waals heterostructures, including 2D-2D and 2D-3D heterostructures. We would like to reveal the basic role of energy, momentum, electronic coupling and excitonic effect on interfacial photoexcitation dynamic processes, to lay the foundation for designing novel and high efficient van der Waals heterostructure devices.

金属半导体界面等离激元增强的热电子过程

谭世谅

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在金属半导体异质结中，激发金属纳米颗粒的局域等离激元共振可以有效的增强半导体材料的光催化效应及光伏性质。等离激元共振增强的热电子是这个过程中的能量载体。通常，异质体系中的热电子过程主要有以下三种形式：一，热电子在金属中激发，然后转移到半导体；二，通过界面的等离激元场耦合而直接在半导体中激发热电子；三，通过特定的共振相干通道实现从金属向半导体的直接激发。长期以来，对这三种过程的表征与调控具有极高的挑战性。通过利用时间分辨的相干多光子光电子能谱，我们从能带结构的角度，研究热电子激发、弛豫、界面电荷转移和能量转移等超快动力学过程。首先从洁净石墨表面入手，发现了Dirac能带中超过8个光子的反常非线性光激发过程[1]；进一步通过构建Ag纳米颗粒/石墨异质结，识别了界面态激发和石墨中π-π* transition这两个主要的热电子来源，并发现这两部分热电子具有完全不同的寿命[2]；通过调控界面态与石墨层间态(interlayer band)之间的共振，实现了电子从Ag向石墨的直接激发，揭示了这一界面电荷转移中的相干行为[3]；在Ag/TiO_2(110)异质结中，发现了平面内的等离激元模式激发的热电子具有各项异性的分布特征，并通过超快时间、能量和空间上的多维光电子谱表征揭示了在小于10飞秒时间尺度内，界面的等离激元耦合及退激发而实现的能量转移过程[4]。

[1] Tan, S. *et al.*, Phys. Rev. X, **7**, 011004 (2017).
[2] Tan, S. *et al.*, J. Am. Chem. Soc., **139**, 6160-6168 (2017).
[3] Tan, S. *et al.*, Phys. Rev. Lett., **120**, 126801 (2018).
[4] Tan, S. *et al.*, Nat. Photon., **11**, 806-812 (2017)

Workshop Information

➢ Arrival and Registration

1. Lobby at the **Anhui Empark Grand Hotel (安徽世纪金源酒店)**

   June 8, 2018

2. Meeting place: **Exhibition Hall in the Hefei National Laboratory Building, USTC**

(中国科学技术大学微尺度国家研究中心一楼科技展厅)

   June 9-10, 2018

➢ Hotel

Anhui Empark Grand Hotel (安徽世纪金源酒店)

Address: 5558 Huizhou Avenue, Binhu New District, Hefei 230042, China

Tel: (86)-551-66868888; Website: www.empark.com.cn/anhui/

➢ Shuttle

Shuttle route	Departure time
Anhui Empark Grand Hotel → USTC	8:25am, June 9, 10
USTC → Anhui Empark Grand Hotel	8:30pm, June 9

➢ Meals

Date	Place
Dinner buffet on June 8	Anhui Empark Grand Hotel (安徽世纪金源酒店)
Lunch buffet on June 9, 10	Faculty Restaurant, USTC (中国科学技术大学教工餐厅)
Banquet on June 9 (By Invitations)	Yueya Jiangnanchun Business Hotel (悦雅江南春商务酒店)

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Brief Introduction

Supported by the University of Science and Technology of China (USTC), the International Center for Quantum Design of Functional Materials (ICQD) was founded in summer 2008 as a cross-divisional research entity within the Hefei National Laboratory for Physical Sciences at the Microscale (HFNL). It aims to advance the frontiers of materials science for quantum information and clean energy, and serves as USTC's important platform for promotion of domestic and international scientific exchanges and collaborations in these and emerging areas. The Center emphasizes synergetic research between theory and experiment, strives for discoveries and establishments of new concepts, and promotes scientific achievements that could benefit the humanity. Initial research focuses of ICQD included quantum transport, quantum magnetism & spintronics, nanoclusters & nanocatalysis, nanoplasmonics, and clean energy. All these thrust areas still lie at the forefronts of today's physics, chemistry, and materials science, and are inherently mutually connected, whose advances are measured by major breakthroughs in basic science, which in turn are expected to have lasting impacts in protecting national interest and promoting world peace. With the development of the Center and the evolution of the relevant disciplines, the research thrusts will also make necessary expansion and adjustment.

在中国科学技术大学的支持下，国际功能材料量子设计中心依托合肥微尺度物质科学国家实验室（筹）于 2008 年夏成立。中心是一个跨学科的研究实体，致力于推动量子信息和清洁能源两大领域的科学前沿研究，同时为中科大在相关领域的国内外学术交流与合作提供一个重要窗口。中心弘扬理论与实验互动性结合的研究文化，侧重于新概念与新学说的发现与建立，并铭记以研究成果造福人类的可行性。中长期目标是凝练发展研究特色，提升科研水平，将中心逐步发展成为具有国际影响力的量子材料基础与应用学术研究重镇。中心初期的研究重心是量子输运，量子磁性及自旋电子学，纳米团簇及纳米催化，纳米等离激元学，以及清洁能源。这五大研究领域均属当今世界物理、化学与材料科学前沿，有很强的交叉性和关联性；其发展既孕育于基础科学的重大突破，又兼具保护国家利益与促进世界和平的前瞻性使命。随着中心的发展与国际上相关学科的演变，中心的主攻方向也将作出相应的扩展与调整。

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