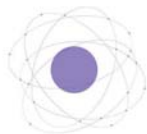


# 第十七届全国化学动力学会议

# 会议手册

主办单位：中国化学会  
承办单位：中国科学技术大学  
协办单位：黄山学院



2022年8月  
安徽·屯溪



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## 参会须知

### ● 温馨提示 ⓘ

🔊 为保证会议顺利进行,请您注意以下事项:

- 1.根据疫情防控需要,请正确佩戴好口罩并配合工作人员做好防疫检查;
- 2.请自觉维护会场秩序,服从大会安排,会议期间如无特殊情况,请勿在会场随意走动;
- 3.请自觉维护环境整洁,会场内禁止抽烟;
- 4.会议期间请将通讯设备关闭或静音状态,如需接听电话请移步至场外;
- 5.请妥善保管好个人财务及重要文件等贵重物品,谨防丢失。

### ● 餐饮服务 ✂

自助餐:昱城皇冠假日酒店一楼玉屏轩餐厅、三楼江畔餐厅

午餐时间:12:00-13:30      晚餐时间:17:30-20:45

桌餐:昱城皇冠假日酒店一楼大宴会厅

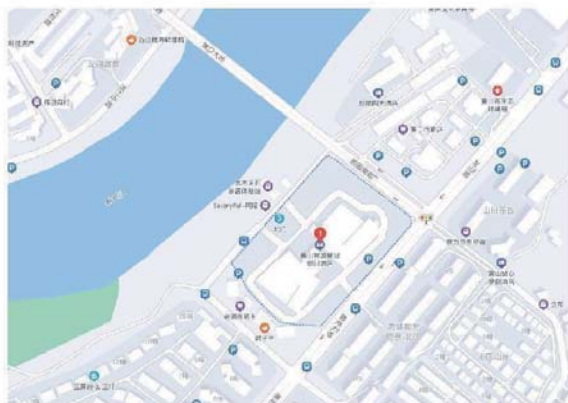
时间:8月24日18:40-20:30

报到时领取餐券,遗失不补,请妥善保管并前往指定地点用餐,大会就餐人数较多,自助餐请错峰用餐,由此带来的不便敬请谅解。

## 参会须知

### 酒店方位示意

宣城皇冠假日酒店(黄山市屯溪区徽州大道1号)



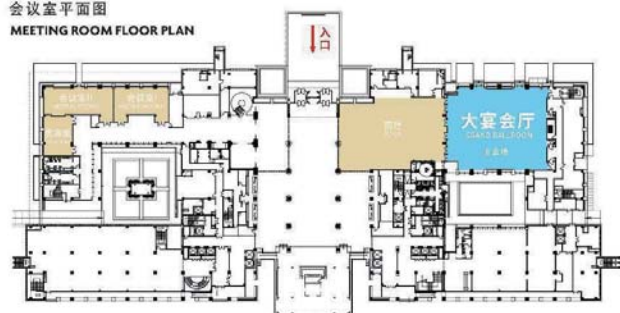
#### 会场周边:

新徽天地醉温泉旅游度假区、柏山法制文化园、黄山园、天盈购物中心、黄山天润发超市等游购娱乐场所,可根据您的行程安排,自行前往。

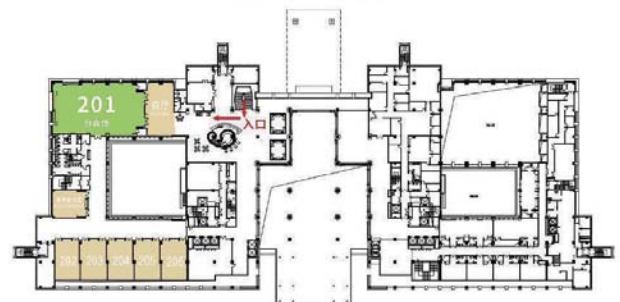
## 参会须知

### 会场信息

会议室平面图  
MEETING ROOM FLOOR PLAN



一楼 会议室平面图  
1st FLOOR MEETING ROOM FLOOR PLAN



二楼 会议室平面图  
2nd FLOOR MEETING ROOM FLOOR PLAN

## 大会组委会

### 学术委员会

主任：杨学明

副主任：张东辉、周鸣飞、边文生、谢代前、苏红梅

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秘书：陈金枚、刘 敏

## 日程安排

### 大会报告

时间：2022年8月24日 09:00-12:00 14:00-18:00

地点：昱城皇冠假日酒店一楼大宴会厅、  
二楼多功能厅201(转播)

### 分会报告(一)

时间：2022年8月25日-2022年8月26日

08:30-12:00 14:00-18:00

地点：昱城皇冠假日酒店一楼大宴会厅

### 分会报告(二)

时间：2022年8月25日-2022年8月26日

08:30-12:00 14:00-18:00

地点：昱城皇冠假日酒店二楼多功能厅201

## 报告摘要

## 特邀报告

## 星际小分子极紫外光化学动力学研究

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分子光化学主要研究分子吸收光子之后旧化学键断裂、新化学键形成以及分子异构化等相关过程。分子光化学在星际科学领域有重要作用。近半世纪以来,分子在紫外波段(200-400nm)的光化学取得了很大的进展,但是在极紫外波段(50-180nm),由于激光光源的缺乏,国内外相关的研究较少。而宇宙早期广泛存在的小分子比如CH<sub>4</sub>、H<sub>2</sub>O、CO<sub>2</sub>、CO、H<sub>2</sub>等,它们的电子吸收谱都在极紫外光谱区域。这些分子的极紫外光化学过程对理解宇宙早期分子演化以及生命的起源有着重要的作用。过去二十多年,我们实验室发展了利用一个混频池产生两束极紫外光的技术,解决了双束极紫外光空间和时间重合较难的问题,将高分辨的氢原子里德堡态飞行时间谱和可调的极紫外光结合起来,开展了系列性的高分辨极紫外光化学动力学研究。近年来,我们实验室进一步发展了基于可调极紫外自由电子激光技术的分子光化学实验方法,研制成功基于极紫外自由电子激光的分子光化学实验站,并集成氢原子平动能谱和离子成像探测技术,实现分子全波段光解离和所有产物通道的探测。本报告介绍利用分子光化学实验新方法,系统研究H<sub>2</sub>O和H<sub>2</sub>S等分子的极紫外光化学动力学以及其在星际化学中的意义。此外,报告还将介绍极紫外自由点激光在其他科学问题研究中的应用。

**关键词:** 极紫外;自由电子激光;光解离

## 参考文献

- [1] Z. J. Luo et al., *Sci. Adv.* 2021, 7, eabg7775.
- [2] Y. Chang et al., *Nat. Commun.* 2021, 12, 2476.
- [3] Y. Zhao et al., *Nat. Commun.* 2021, 12, 4459.
- [4] Y. Chang et al., *Nat. Commun.* 2021, In revision.
- [5] J. M. Zhou et al., *Nat. Commun.* 2020, 11, 1547.
- [6] Y. Chang et al., *Nat. Commun.* 2019, 10, 1025.

## 报告摘要

## 特邀报告

## Simulating ultraviolet-visible absorption spectra of polyacenes and X-ray absorption spectra of carbon monoxide on a superconducting quantum processor

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Here, we describe a pragmatic hybrid quantum-classical approach more suitable for NISQ (Noisy Intermediate-Scale Quantum) devices, termed the variational quantum response (VQR) approach.<sup>1</sup>We implement it on a state-of-the-art superconducting quantum processor with all-to-all qubit connectivity to realize the first ever quantum computation of linear optical properties of molecules. The feasibility of VQR is benchmarked for computing dynamic polarizabilities of the hydrogen molecule (H<sub>2</sub>) at three geometries with different electron correlation strengths.<sup>2</sup> We then apply it to tackle two representative problems of practical significance, viz., simulating ultraviolet-visible absorption spectra of polyacenes and X-ray absorption spectra of carbon monoxide.<sup>3</sup> These results represent an initial step towards exploring quantum computing for reliably simulating linear and nonlinear response properties of more challenging systems in the near future.

**Acknowledgements:** This work has the support of the National Natural Science Foundation of China (Grant No: 22288201)

## References

- [1] X. Cai, W.-H. Fang, H. Fan, and Z. Li, Quantum computation of molecular response properties. *Phys. Rev. Research* 2: 033324 (2020)
- [2] X. Cai, Z. Li, H. Fan, and W.-H. Fang, Simulating linear optical properties of molecules on a superconducting quantum processor (unpublished)

## 报告摘要 特邀报告

## 从超冷化学反应到体相水的第一性原理模拟

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分子反应动力学国家重点实验室

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报告将介绍最近几年我们在超冷量子散射以及体相水多体势能面研究上的一些进展。随着超冷物理/化学研究的不断发展,超冷条件下的分子碰撞反应越来越受到关注。目前的超冷量子散射研究都利用传统的非含时方法,只能处理三原子反应。利用含时波包法处理更大的超冷反应需要克服两个问题:1. 超冷反应非常长的德布罗意波长所带来的吸收问题;2. 超冷反应的低速运动所引起的长时间传播问题。报告将介绍我们在克服这两个问题上所发展的新方法以及一些应用。

体相水的计算模拟需要高精度的水分子相互作用势能面(力场)。自50年前首次对体相水进行计算模拟以来,水分子力场构造取得了巨大的进展,但发展一个能够精确描述水从气体、团簇到凝聚相行为的分子模型仍面临巨大挑战。在过去的十年中,基于置换不变多项式(PIP)拟合的水分子二体、三体、甚至四体的相互作用势能面被广泛应用于水团簇和体相水的理论研究。本报告将介绍我们最近几年使用基本不变神经网络(FI-NN)构造二体、三体、四体水分子相互作用势能面的进展,以及基于这些多体相互作用势能面所取得一些水团簇和体相水的模拟结果。

## 报告摘要 特邀报告

## 复杂分子体系的相互作用及动力学模拟

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We will discuss some recent progress in computational study of complex molecular systems. These include new approaches that combine quantum chemistry calculation, machine learning and molecular dynamics to simulate complex chemical reaction processes in which hundreds of chemical reactions occur simultaneously. The new approach allows one to simulate real chemical reactions processes, trace individual reaction paths and discover new reactions without the prior knowledge of specific reactions. We will also discuss how accurate quantum chemistry calculations can be extended to biomolecules by using fragment quantum approach.

## References

1. Cao, et al., *Molecules*, 2021, 26, 3120.
  2. Xu, et al., *Front. Chem.*, 6, 189, (2018).
  3. Xu, et al., *J. Phys. Chem. A*, 123, 6587–6595 (2019).
  4. Jinzhe Zeng, et al., *Nature Communications*, 2020, 11, 5713.
- [2] F. L. Author, H.-G. Test, book title (publishing company, place, year).



## 报告摘要

## 邀请报告

## 分子的腔增强振动激发与精密测量

程存峰, 胡水明\*

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腔增强光谱技术是近几年发展起来的灵敏光谱探测手段, 在大气分子光谱探测、精密光谱测量、反应物激发和产物探测等方面具有广泛应用。结合精密激光锁频和频率控制技术, 我们发展了新的腔增强振动激发与精密测量技术。利用腔增强振动激发技术, 实现了对CO、CO<sub>2</sub>分子激发态的精密光谱测量, 并将该技术应用于分子同位素的痕量检测。未来有望在分子束流中实现分子的高效率激发和检测, 为激发态化学反应研究提供技术支持。基于激光锁频的腔增强光谱方法, 实现了对HD分子微弱振动跃迁的精密测量。测量中发现, HD微弱的振动跃迁非常容易受到强电子跃迁的扰动, 产生非对称线形。结合量子光学计算, 对HD分子的非对称线形进行分析, 获得了10位数有效数字的跃迁频率测量精度。未来有望在分子束中实现HD分子高效率激发和精密光谱测量, 结合高精度的量子力学理论, 可以精确测量质子-电子质量比等基本物理常数。

## 参考文献

- [1] J. Wang, etc., Journal of Chemical Physics, 147: 091103 (2017)
- [2] L.-G. Tao, etc., Physical Review Letters, 120: 153001 (2018)
- [3] T.-P. Hua, etc., Optics Letters, 45(17): 4863 (2020)
- [4] C.-L. Hu, etc., Journal of Physical Chemistry Letters, 11: 7843-7848 (2020)
- [5] Y.-D. Tan, etc., Chinese Journal of Chemical Physics, 34(4): 373-380 (2021)

## 报告摘要

## 邀请报告

## Generalized Surface-Hopping Carrier Dynamics Simulations: Spin-Orbit Effects on Electronic Properties of Perovskites

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Two-dimensional (2D) perovskites are emerging as promising candidates for diverse optoelectronic applications because of low cost and excellent stability. Recently, we explore the electronic structures and interfacial properties of (4Tm):PbI<sub>3</sub> with both the collinear and noncollinear DFT (PBE and HSE06) methods. The results evidently manifest that explicitly considering the spin-orbit coupling (SOC) effects is necessary to attain correct band alignment of (4Tm):PbI<sub>3</sub> that agrees with recent experiments very well (Nat. Chem. 2019, 11, 1151; Nature 2020, 580, 614). The subsequent time-domain noncollinear DFT-based nonadiabatic carrier dynamics simulations with the SOC effects reveal that the photoinduced electron and hole transfer processes are asymmetric and associated with different rates. The differences are mainly ascribed to considerably different nonadiabatic couplings in charge of the electron and hole transfer processes. Shortly, our current work sheds important light on the mechanism of the interfacial charge carrier transfer processes of (4Tm):PbI<sub>3</sub>. The importance of the SOC effects on correctly aligning the band states of (4Tm):PbI<sub>3</sub> may be generalized to similar organic-inorganic hybrid 2D perovskites having heavy Pb atoms.



Figure 1: The inclusion of spin-orbit coupling changes the interfacial properties of perovskites.

## References

- [1] J.J. Yang, W.K. Chen, X.Y. Liu, W.H. Fang, and G.L. Cui\*, JACS Au, 2021, 1, 1178.
- [2] X.Y. Liu, J.J. Yang, W.K. Chen, X.Y. Liu, A.V. Akimov, W.H. Fang, and G.L. Cui\*, J. Phys. Chem. Lett., 2021, 12, 1131.

## 报告摘要

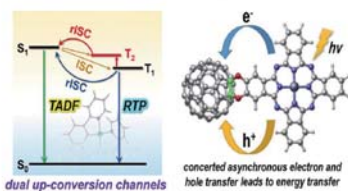
## 邀请报告

## 复杂体系非绝热过程的理论与计算模拟

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非绝热过程普遍存在于物理、化学、生物、材料等诸多领域, 且在其中发挥着重要作用。探索其微观本质对生命过程、光电功能材料和新能源的开发都具有重要意义。其中, 光化学体系具有最丰富的非绝热过程, 其动力学错综复杂, 其机理探索更是极具挑战。近年来, 针对复杂体系不同时间尺度的非绝热过程, 课题组发展了一系列精准、高效的计算模拟方法, 并采用发展的方法研究了一些重要的非绝热过程, 提出了新模型, 揭示了微观本质。在本报告中, 我将主要汇报课题组在这方面的理论工作。



## 参考文献:

- [1] Cui, G.L. et al. Chemistry-A European Journal, 27, 4159-4167 (2021).
- [2] Cui, G.L. et al. Journal of Physical Chemistry Letters, 12, 5944-5950 (2021).
- [3] Cui, G.L. et al. Journal of Physical Chemistry C, 125, 27372-27380 (2021).
- [4] Cui, G.L. et al. Inorganic Chemistry, 61, 7673-7681 (2022).
- [5] Cui, G.L. et al. Chemistry-A European Journal, in press (2022).

## 报告摘要

## 邀请报告

## 分子非共价相互作用与分子同分异构的质谱分析

吴芳玲<sup>1</sup> 戴新华<sup>2</sup> 方向<sup>1</sup> 丁传凡<sup>1\*</sup><sup>1</sup>宁波大学质谱研究院, 浙江省先进质谱技术与分子检测重点实验室<sup>2</sup>中国计量科学研究院

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分子同分异构体的化学结构及其功能一直受到重视, 这是由于异构体分子可能具有完全不同的生物化学活性, 如同分异构体的某个分子对疾病发病机理或疾病治疗具有重要的作用。因此, 对同分异构体的分离识别及其结构的探究, 有助于进一步理解药物作用和生命功能机制。由于同分异构体之间各种物理化学性质的高度相似性, 使得传统的光谱, 质谱, 核磁等分析方法在分析分子的同分异构体方面都存在这样或那样的困难。近年来快速发展起来的离子迁移谱 (Ion mobility spectrometry, IMS) 是一种可以分析分子空间结构的仪器技术, 它通过测量气相中不同分子离子的碰撞截面来区分某种分子的同分异构体。IMS与质谱联用技术 (IMS-MS) 是一种强大的分离分析技术, 即在质谱技术上增加了一个滴度分离维度改善离子结构分离测定, 同时也在滴度的技术上增强离子选质的特殊功能, 使分析离子的分离具有高度选择性。本工作通过合成分子同分异构体的非共价复合物, 实现分子空间结构的变化, 然后利用质谱和离子迁移谱分析获得分子同分异构体的空间结构信息。分子结构的理论计算结果与实验结果基本吻合。

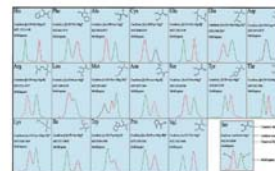


图1 19组手性氨基酸对映体的质谱-离子迁移谱分析结果

## References

- [1] Yang S, Gu L, Wu F, Dai X, Xu F, Li Q, Ding C F. Talanta, 2022, 243: 123363.
- [2] Yang S, Wu F, Yu F, Gu L, Wang H, Liu Y, Ding C F. Analytica Chimica Acta, 2021, 1184: 339017.
- [3] Wang H, Wu F, Xu F, Liu Y, Ding C F. Analytical Chemistry, 2021, 93(45): 15096-15104.



## 报告摘要

## 邀请报告

## Vibrationally resolved optical images

Sai Duan<sup>1\*</sup>, Guangjun Tian<sup>2</sup>, and Yi Luo<sup>3</sup><sup>1</sup>Department of Chemistry, Fudan University, Shanghai 200433.<sup>2</sup>Department of Physics, Yanshan University, Qinhuangdao 066004.<sup>3</sup>Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, 230026.

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One of the most important dynamics in chemistry is the motions of electrons and atomic nuclei in molecules. Motivated by the spirit of "seeing is believing", observing these motions as well as their coupling in real space via optical means is the ultimate dream in chemistry. However, owing to the diffraction limit, it is even impossible to see typical molecules with a size scale around nanometer by far-field optical techniques in the visible region.

In this report, we will focus on molecular responses of highly confined near-fields. In this context, it has been experimentally demonstrated that optical images have the ability for observing inner molecular structures[1]. A fully quantized electrodynamic theory was established, in which spatial distributions of near-field can be rigorously taken into account[2]. The new theory reveals that experimentally observed super-high resolution of resonant Raman scattering images is related to the electronic transitions between ground and resonant electronic excited states and thus are insensitive to the atomic motions[2]. To obtain the optical images involving atomic motions, the new theory manifests that the Herzberg-Teller contribution has to be promoted. The first theoretical prediction is the nonresonant Raman images[3], where the Herzberg-Teller contribution is naturally enhanced. Our numerical results reveal that the non-resonant Raman images can faithfully visualize the atomic motions of molecular vibrations in real space, which has been confirmed by recent experiments. We will further discuss the other two vibrationally resolved optical images. One of them is tip-enhanced fluorescence excitation spectroscopy, where Kasha's rule plays an essential role. Another one is a special case in resonant Raman scattering images, where the advantage of the extremely long lifetime of excited states is highlighted. Both vibrationally resolved images have the ability to visualize the coupling between motions of electrons and nuclei in molecules.

**Acknowledgements:**

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**References**

- [1] Zhang et al., Nature, 498, 82 (2013).
- [2] Duan et al., J. Am. Chem. Soc., 137, 9515 (2015).
- [3] Duan et al., Angew. Chem. Int. Ed., 55, 1041 (2016).

## 报告摘要

## 邀请报告

## Highly accurate potential energy surfaces and dynamics of chemical reactions with up to 15 atoms

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Symmetry adaptation is crucial in representing a permutationally invariant potential energy surface (PES). We developed the efficient fundamental invariant-neural network (FI-NN) approach to construct PESs with permutation symmetry with high accuracy. It is fascinating that the applicable size has now been pushed up to systems of more than 10 atoms. We have developed accurate PESs for complicated prototype reactions in combustion chemistry and gas-phase organic chemistry. Dynamics simulations based on these PESs reveal novel and interesting reaction mechanisms at the atom-molecular level, which can further provide deep insight into the understanding of dynamics in combustion chemistry and organic chemistry.

Figure 1: Schematic PES of the F + (CH<sub>3</sub>)<sub>2</sub>Cl reaction.

**Acknowledgements:** This work has the support of the National Natural Science Foundation of China.

**References**

- [1] X. Lu, C. Shang, L. Li, R. Chen, B. Fu\*, X. Xu, D. H. Zhang\*, Nat. Comm., accepted.
- [2] X. Lu, L. Li., X. Zhang, B. Fu\*, X. Xu., D. H. Zhang\*, J. Phys. Chem. Lett. 13, 5253(2022).
- [3] Y. Fu, Y. Bai, Y. Han\*, B. Fu\*, D. H. Zhang, J. Phys. Chem. Lett., 12, 4211(2021).
- [4] Y. Fu, X. Lu, Y. Han\*, B. Fu\*, D. H. Zhang\*, J. M. Bowman\*, Chem. Sci., 11, 2148 (2020).
- [5] Y. Hong, Z. Yin, Y. Guan, Z. Zhang, B. Fu\*, D. H. Zhang\*, J. Phys. Chem. Lett. 11, 7552(2020).

## 报告摘要

## 邀请报告

## Site-Specific Interrogation of Protein Conformation and Dynamics

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The structural integrity of a folded protein is maintained by a number of weak interactions so it can undergo various local and global fluctuations. In addition, a protein may be intrinsically disordered, sampling a dynamic conformational ensemble without forming well-defined and long-lasting tertiary contacts. Moreover, for performing its function a protein may possess a certain degree of structural plasticity. Therefore, in order to yield a microscopic understanding of the conformational energy landscape and the underlying structure-dynamics-function relationship of the protein in question, it is necessary to acquire the needed information at individual amino acid level. However, it is not easy or even feasible to obtain such information via commonly used spectroscopic techniques as native spectroscopic signals often lack the required structural and/or spatial resolutions. In this talk, we will discuss our ongoing efforts to overcome this limitation. In particular, we will describe several examples, showing how unnatural amino acid-based spectroscopic probes can be used to reveal protein electric field, solvent accessibility, conformation, and conformational dynamics in a site-specific manner.

## 报告摘要

## 邀请报告

## 量子态选择的离子-分子散射动力学研究

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离子与分子之间的碰撞反应及能量传递过程对行星大气、星际物质、等离子体以及燃烧过程等复杂气相环境的物化性质及演化有重要的影响。研究离子与分子之间的散射动力学需要研制复杂的仪器装置，是分子反应动力学领域最重要的方向之一，具有悠久的历史。基于离子速度成像的交叉分子束技术在中性基元反应动力学研究中取得了巨大的成功，但专门用于研究离子-分子散射动力学的交叉束装置则相对较少。报告人在中科院化学所搭建了一套基于三维离子速度成像技术的离子-分子交叉束装置，并利用激光电离技术产生处于特定量子态的离子，实现量子态选择的离子-分子散射动力学研究[1, 2]。本报告将介绍我们利用该装置研究的第一个反应，即经典的电荷转移反应 $\text{Ar}^+(\text{P}_{1/2}) + \text{N}_2 \rightarrow \text{Ar} + \text{N}_2^+(\text{v})$ 。我们用共振增强多光子电离技术制备处于特定自旋-轨道态的 $\text{Ar}^+(\text{P}_{3/2})$ 和 $\text{Ar}^+(\text{P}_{1/2})$ 离子束，用高分辨三维离子速度成像装置获得具有振动能级分辨的产物 $\text{N}_2^+(\text{v})$ 离子的散射图谱(如图-1所示)，并结合文献报道的结果，对其具有自旋-轨道依赖的电荷转移动力学进行分析和讨论。另外，我们还首次获得其非弹性散射过程的微分散射截面，获得其碰撞能量传递的相关信息。

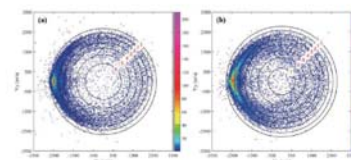


Figure 1: (a)  $\text{Ar}^+(\text{P}_{3/2}) + \text{N}_2 \rightarrow \text{Ar} + \text{N}_2^+(\text{v})$  and (b)  $\text{Ar}^+(\text{P}_{1/2}) + \text{N}_2 \rightarrow \text{Ar} + \text{N}_2^+(\text{v})$  in the collision energy of 1.57 eV of the differential scattering cross-section.

## References

- [1] GD.Zhang, H. Gao, etc. *Chin. J. Chem. Phys.* 34, 71 (2021).
- [2] GD.Zhang, H. Gao, etc. *Rev. Sci. Instrum.* 92, 113302 (2021).

## 报告摘要 邀请报告

## Dynamics and Pathways of an Oxidative Combustion from Direct Molecular Dynamics

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Traditionally, the study of reaction mechanisms of complex reaction systems such as combustion has been performed on an individual basis by optimizations of transition structure and minimum energy path or by reaction-dynamics trajectory calculations for one elementary reaction a time. It is effective, but time-consuming, whereas important and unexpected processes could have been missed. In this presentation, we will discuss a direct molecular dynamics (DMD) approach and the simulation program, CARNOT, in which all possible chemical reactions are simulated simultaneously at finite temperature and pressure conditions. A key concept of the fragment localized ab-initio molecular electronic structure method is to partition a large, chemically reactive system into molecular blocks on the fly in a dynamics simulation. The theory is called reactive explicit polarization (ReX-Pol) for reactive events. We fully explore the local nature of molecular properties in ReX-Pol, rather than treating the entire system by a delocalized wave function such as that in conventional ab initio molecular dynamics (AIMD). Consequently, the DMD approach can be applied to reactive systems consisting of an arbitrarily varying number of closed and open-shell species such as free radicals, zwitterions and separate ions found in combustion and other reactions. Employing the PW91 density functional theory and the 6-31+G(d) basis set, we will illustrate the capabilities of the CARNOT program by a combustion reaction consisting of more than 28,000 atoms. The trajectories reveal a range of mechanistic and dynamical events. Potential applications and improvements will be discussed.

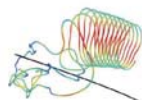


Figure 1: Roaming and ro-vibration dynamics of a collision induced decomposition.

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[2] F. L. Author, H.-G. Test, book title (publishing company, place, year).

## 报告摘要 邀请报告

Rotational insights into  $\pi$  interactions

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A great deal of attention has been given to noncovalent interactions (NCIs) involving  $\pi$  systems because of their widespread presence in biology as well as materials, where they are pivotal in determining the three-dimensional structures of, e.g., proteins and polymers or the selectivity of molecular affinity. Despite dramatic advances in our understanding over past decades, many aspects of NCIs of  $\pi$  systems have only recently been discovered, with many questions remaining. Rotational spectroscopy is arguably the most accurate high-resolution molecular spectroscopic technique due to its high sensitivity to mass distributions of molecules and molecular complexes. The inherent spectral feature with molecular fingerprint stems from the fact that even subtle differences in mass distribution (arising from isotopic substitution, isomerization, tautomerization or conformerization) can lead significant changes in the pattern of rotational transitions. Since the interaction sites and the relative arrangement of moieties can be determined without environmental bias, the method allows identifying the intermolecular forces at play. In this talk, with the recent results we have obtained about NCIs involving  $\pi$  systems [1-4], the possibilities and challenges in rotational studies of molecular complexes will be presented.

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## References

- [1] J. Wang, L. Spada, J. Chen, S. Gao, S. Alessandrini, G. Feng, C. Puzzarini, Q. Gou, J.-U. Grabow, V. Barone, *Angew. Chem., Int. Ed.*, 58 13935-13941 (2019).
- [2] Y. Zheng, S. Herbers, Q. Gou, W. Caminati, J.-U. Grabow, *J. Phys. Chem. Lett.* 12 3907-3913(2021).
- [3] H. Wang, J. Chen, C. Duan, X. Xu, Y. Zheng, J.-U. Grabow, Q. Gou, W. Caminati, *J. Phys. Chem. Lett.* 12 5150-5155 (2021).
- [4] H. Wang, J. Chen, Y. Zheng, D. Obenchain, X. Xu, Q. Gou, J.-U. Grabow, W. Caminati, *J. Phys. Chem. Lett.* 13 149-155 (2022).

## 报告摘要

## 邀请报告

## Towards accurate simulation of complex systems

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To study the complex molecular systems beyond the system size that the current state-of-the-art wavefunction theory methods could handle, fragment-based quantum chemistry approaches have been developed over the past years, and proved to be efficient in dealing with large molecular systems at various ab initio levels. According to the fragmentation approach, the complex molecular system can be divided into subsystems (fragments), and subsequently the property of the whole system can be approximately obtained by taking a proper combination of the corresponding terms of individual fragments. Therefore, the standard quantum chemistry calculation of complex system can be circumvented by carrying out a series of calculations on small fragments, which could significantly promote computational efficiency. The electrostatically embedded generalized molecular fractionation with conjugate caps (EE-GMFCC) method is one of the fragment-based quantum chemical approaches, which has been developed in our research group in recent years. This talk will present the theoretical framework of this fragmentation method and its applications in biomolecules, molecular clusters, molecular crystals and liquids, including total energy calculation, protein-ligand/protein binding affinity prediction, geometry optimization, vibrational spectrum simulation, ab initio molecular dynamics simulation, and prediction of excited-state properties.

## 报告摘要

## 邀请报告

## 中性团簇红外光谱研究

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研究团簇结构与性能随尺寸变化的规律, 对深刻认识和理解物质从分子态到凝聚态的渐变过程具有重大意义。目前, 离子团簇由于带有电荷, 易于探测和质量选择, 研究最为广泛。中性团簇由于缺乏电荷, 难于探测和质量选择, 实验研究非常困难。鉴于上述情况, 我们发展了基于大连极紫外自由电子激光的中性团簇红外光谱实验装置, 实现了质量选择中性团簇的高灵敏探测、结构表征和性能研究[1,2]。利用该方法, 发现了最小水滴立体结构是由5个水分子组成, 打破了前人对最小水滴是由6个水分子的认识, 为理解水的微观结构演化机制提供了新的思路。在本报告中, 首先介绍这个实验方法, 然后举例说明它在中性大气团簇结构及演化机制研究中的应用[3-6]。



## 参考文献:

- [1] G. Li, C. Wang, Q. Li, H. Zheng, T. Wang, Y. Yu, M. Su, D. Yang, L. Shi, J. Yang, Z. He, H. Xie, H. Fan, W. Zhang, D. Dai, G. Wu, X. M. Yang, L. Jiang\*, *Rev. Sci. Instrum.*, 2020, 91, 034103.
- [2] B. Zhang, Y. Yu, Z. Zhang, Y. Zhang, S. Jiang, Q. Li, S. Yang, H. Hu, W. Zhang, D. Dai, G. Wu, J. Li\*, D. H. Zhang\*, X. M. Yang\*, L. Jiang\*, *J. Phys. Chem. Lett.*, 2020, 11, 851.
- [3] B. Zhang, Y. Yu, Y. Zhang, S. Jiang, Q. Li, H. Hu, G. Li, Z. Zhao, C. Wang, H. Xie, W. Zhang, D. Dai, G. Wu, D. H. Zhang, L. Jiang\*, J. Li\*, X. M. Yang\*, *Proc. Natl. Acad. Sci.*, 2020, 117, 15423.
- [4] G. Li, Y. Zhang, Q. Li, C. Wang, Y. Yu, B. Zhang, H. Hu, W. Zhang, D. Dai, G. Wu, D. H. Zhang, J. Li\*, X. M. Yang\*, L. Jiang\*, *Nat. Commun.*, 2020, 11, 5449.
- [5] S. Jiang, M. Su, S. Yang, C. Wang, Q. Huang, G. Li, H. Xie, J. Yang, G. Wu, W. Zhang, Z. Zhang\*, J. L. Kuo\*, Z. F. Liu\*, D. H. Zhang, X. M. Yang, L. Jiang\*, *J. Phys. Chem. Lett.*, 2021, 12, 2259.
- [6] Y.-Y. Zhang, C. Wang, G. Li, X. Zang, Y. Yu, H. Hu, J. Yang, W. Zhang, D. Dai, G. Wu, L. Jiang\*, X. M. Yang\*, J. Li\*, *Cell Rep. Phys. Sci.*, 2022, 3, 100748.
- [7] C. Wang, L. Fu, S. Yang, H. Zheng, T. Wang, J. Gao, M. Su, J. Yang, G. Wu, W. Zhang, Z. J. Zhang\*, G. Li\*, D. H. Zhang, L. Jiang\*, X. M. Yang, *J. Phys. Chem. Lett.*, 2022, 13, 5654-5659.
- [8] F. L. Author, H.-G. Test, book title (publishing company, place, year).



## 报告摘要

## 邀请报告

## 高振动激发态分子在金属表面散射的绝热与非绝热动力学

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气固界面的化学反应是多相催化、晶体生长、金属腐蚀等表面物理化学过程中重要的基元步骤, 伴随着不同自由度之间的能量转换。因此, 理解分子在固体表面的内部能量重新分布以及分子与表面之间的能量交换对理解这些复杂的表面现象至关重要。与气相反应相比, 气相-表面体系自由度显著增大, 其动力学微观机制的理论描述面临着巨大挑战。近年来, 我们聚焦于发展通用的嵌入原子神经网络方法, 实现了包含分子和表面原子自由度的高维势能面以及金属表面分子电子摩擦张量的精确构造, 进而研究了高振动激发分子在金属表面散射的绝热和非绝热传动力学, 揭示了分子与金属表面振动传能与解离过渡态附近的势能面形貌之间的深刻联系。在此基础上, 我们也取得了关于分子与金属表面电荷转移动力学的初步结果。

## 参考文献

- [1] R. Yin, Y. Zhang, and B. Jiang, *J. Phys. Chem. Lett.* 10, 5969 (2019).
- [2] Y. Zhang, R. J. Maurer, and B. Jiang, *J. Phys. Chem. C* 124, 186 (2020).
- [3] R. Yin, and B. Jiang, *Phys. Rev. Lett.* 126, 156101 (2021).
- [4] C. L. Box, Y. Zhang, R. Yin, B. Jiang, and R. J. Maurer, *JACS Au* 1, 164 (2021).
- [5] Y. Zhang, J. Xia, and B. Jiang, *Phys. Rev. Lett.* 127, 156002 (2021)
- [6] G. Meng, C. Hu, and B. Jiang *J. Phys. Chem. C* 126, 12003 (2022)

## 报告摘要

## 邀请报告

## Electric-Pumped Transient Absorption Spectroscopy

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Similar as in the photoinduced processes in solar cell or photocatalysis, there also exists complicated carrier or charge dynamics and subsequent reactions in electroluminescence (EL) and electrocatalytic (EC) materials. However, because of the lack of suitable spectroscopic technique, the study of electric-induced charge dynamics in such materials encounters significant challenges. Many key scientific questions, such as how the external charges inject into the materials and what is the subsequent charge behaviors and the charge transfer induced chemical intermediate, are yet unclear. In this report, we will introduce the development of a newly time-resolved spectroscopy by combining the electric-pulse generator with traditional transient absorption/reflection spectroscopy and its application in revealing the electron injection dynamics in quantum dot LEDs. This technique will be also applied in the study of charge dynamic in other typical EL and EC materials. The results will enlighten electric-induced charge dynamic/mechanism and thus provide essential fundamentals for the development of highly efficient EC and EL materials and devices.

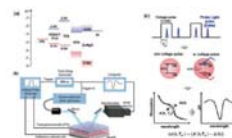


Figure 1: (a) Structure and energy diagram of QLEDs used in this work; (b) Setup of electric-pumped transient absorption (E-TA) method. (c) Principles of electric-pumped transient absorption (E-TA) method.



## 报告摘要 邀请报告

## Methodology development and applications of multi-scale molecular modeling and simulations of complex biosystems

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Given the large ensembles of structures constructed by the essential components like amino acids and nucleotides, their diverse conformations and corresponding interactions with surrounding key small molecules have become challenging to study in various biosystems. Although experimental tools have obtained helpful information, the assistance of probe molecule or atomic force may also bring in bias and errors to understand real biological phenomena. With the emerging use of computational studies, it has yielded mechanistic details of fundamental processes unavailable through experiments alone. Nevertheless, current molecular modeling and simulation techniques meet their limits to accomplish both high resolution and low cost in resolving large complex biosystems, parts of which are due to the methodology. In last decades, we have achieved significant progresses in developing methodologies with improved accuracy and efficiency, which have been applied and provided insights in structure-function relationships and drug development in various biological and medical fields.

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## References

- [1] X. Wang, et al. G.H. Li, W.W. Yang, Nature 571 127(2019).
- [2] P. Lan, M. Tan, G.H. Li, M. Lei, Science 362 6678 (2018).
- [3] Q. Zhong, G.H. Li, J. Phys. Chem. Lett. 12 3151-3162 (2021).
- [4] A. Wang, et al. G.H. Li, J. Phys. Chem. Lett. 11(1), 325 (2020)
- [5] X. Peng, et al. G.H. Li, J. Chem. Theory Comput. 14(3) 1216 (2018)

## 报告摘要 邀请报告

## Constructing high-accurate PES by machine learning model with physical insight and symmetry consideration

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The potential energy surface (PES) is one of the prerequisites for nearly all atomic-scale simulations, and the accuracy and efficiency of the given PES determine the accuracy and cost of calculating further physical quantities. Nowadays, many machine learning (ML) PES models, especially neural network (NN) PES, have been developed and become more and more popular due to their convenience in the application and the functional universality in high-dimensional function fitting. However, compared to physics-motivated models, the general machine learning PES models usually need more fitting points to "learn" the correct asymptotic behavior and have bad extrapolation outside the dataset region. Moreover, without rigorous symmetry consideration, the ML model can hardly preserve the symmetry of the system. For diabatic potential energy matrix (DPEM) fitting, the permutation anti-symmetry will be troublesome if the system becomes large. [1].

In this presentation, we will illustrate our recent development on 1. the physics-based machine learning model for inter-molecular PES fitting, and 2. the permutation-symmetry-adapted ML model for DPEM fitting. The first ML model, named MLRNet, combines the neural network model and the Morse/Long-Range (MLR) function. The physically realistic behavior of the MLR function ensures the MLRNet has meaningful extrapolation at both short and long ranges, which solves the asymptotic extrapolation problem in common neural network potential (NNP) models. The second ML model can approximate both permutation-symmetric and anti-symmetric elements on the meanwhile by constructing the equivariant neural network (ENN).

Thus, permutation-symmetry of the boson-fermion mixture wave function or the DPEM of the non-degenerate electronic states can be rigorously preserved. We further combined the ENN model with the machine learning diabatization method, and construct the first global DPEM of the MgH<sub>2</sub> 1A' and 2A' state [2].

## References

- [1] You Li, Yu Zhai, Hui Li\*, to be submitted (2022)
- [2] You Li, Hui Li\*, et al., J. Chem. Phys., 155, 214102 (2021)

## 报告摘要

## 邀请报告

## Nano-Catalysis or Dynamic Single-Atom Catalysis?

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Catalysis science is essential for chemical industries, environment, energy, human health, biological transformation, and atmospheric processes. In recent years, heterogeneous single-atom catalysts (SAC) have aroused significant interest in the catalysis community [1-3]. Based on ab initio molecular dynamics simulations of  $\text{Au}_{20}/\text{TiO}_2$  and  $\text{Au}_{20}/\text{CeO}_2$  nanocatalysts, we have revealed that the microscopic mechanisms of a series of nano-scale catalytic reactions involve dynamic single-atom catalysts (DSAC), which account for the activity and size-effect of metal catalysis, esp. gold catalysis [4-7]. In this talk, we will show that nanocatalysis often involves DSACs, a fact that is overlooked for a long time. We will discuss our recent theoretical results on the computational studies relevant to DSAC and provide an overview of heterogeneous single-cluster catalysts (SCC) [8-10].

## References

- [1] (a) B. Qiao, A. Wang, X. Yang, L. F. Allard, Z. Jiang, Y. Cui, J. Liu, J. Li, T. Zhang, "Single-Atom Catalysis of CO Oxidation Using Pt1/FeOx", *Nature Chem.* 3 (2011) 634. (b) X. Yang, A. Wang, B. Qiao, J. Li, J. Liu, T. Zhang, "Single-Atom Catalysts: A New Frontier in Heterogeneous Catalysis", *Acc. Chem. Res.* 46 (2013) 1740. (c) A. Wang, J. Li, T. Zhang, "Heterogeneous Single-Atom Catalysis", *Nat. Rev. Chem.* 2 (2018) 65.
- [2] (a) Y.-G. Wang, Y. Yoon, V.A. Glezakou, J. Li, R. Rousseau, "The Role of Reducible Oxide-Metal Cluster Charge Transfer in Catalytic Processes: New Insights on the Catalytic Mechanism of CO Oxidation on Au/TiO<sub>2</sub> from Ab Initio Molecular Dynamics", *J. Am. Chem. Soc.* 135 (2013) 10673. (b) Y.-G. Wang, D.-H. Mei, V.-A. Glezakou, J. Li, R. Rousseau, "Dynamic Formation of Single-Atom Catalytic Active Sites on Ceria-Supported Gold Nanoparticles", *Nature Commun.* 6 (2015) 6511.
- [3] (a) J.-C. Liu, Y.-G. Wang, J. Li, "Toward Rational Design of Oxide-Supported Single Atom Catalysts: Atomic Dispersion of Gold on Ceria", *J. Am. Chem. Soc.* 139 (2017) 6190. (b) Y. He, J.-C. Liu, L. Luo, Y.-G. Wang, J. Zhu, Y. Du, J. Li, S. X. Mao, C. Wang, "Size-Dependent Dynamic Structures of Supported Gold Nanoparticles in CO Oxidation Reaction Condition", *Proc. Natl. Acad. Sci. USA.* 115 (2018) 7700.
- [4] (a) S. Zhang, L. Nguyen, J.-X. Liang, J. Shan, J. Liu, A. I. Frenkel, A. Patlolla, W. Huang, J. Li, F. Tao, "Catalysis on Singly Dispersed Bimetallic Sites", *Nature Commun.* 6 (2015) 7938. (b) X.-L. Ma, J.-C. Liu, H. Xiao, J. Li, "Surface Single-Cluster Catalyst for N<sub>2</sub>-to-NH<sub>3</sub> Thermal Conversion", *J. Am. Chem. Soc.* 140 (2018) 46. (c) J.-C. Liu, X.-L. Ma, Y. Li, Y.-G. Wang, H. Xiao, J. Li, "Heterogeneous Fe<sub>2</sub> Single-Cluster Catalyst for Ammonia Synthesis via an Associative Mechanism", *Nature Commun.* 9 (2018) 1610. (c) Z. Lin, M. E.-Escribano, J. Li, "Recent Progress and Perspectives on Single-Atom Catalysis", *J. Mater. Chem. A* 10 (2022) 5670.

## 报告摘要

## 邀请报告

## 有机单晶和纳米晶激发态和瞬态中间体的超快光谱探测与调控

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超快时间分辨光谱是研究光诱导引起的光物理、光化学、光生物和光药物等的超快过程反应机制的最重要的研究手段。光功能材料的激发态是高能的活性中间体, 寿命短、电子结构异常复杂, 导致其光物理和光化学过程难以控制。光功能材料激发态的时空探测与调控尚处在起步阶段, 是目前光化学领域研究的热点和难点。通过超快光谱研究复杂的光物理和光化学过程, 跟踪和探测激发态和瞬态中间体, 获得激发态和瞬态中间体电子结构和动力学过程是理解复杂光化学光控机制的基础, 但难以实现。实际器件设计中, 有机光功能材料通常以固体样品形式存在。而固体样品激发态和瞬态中间体的光谱探测与动力学研究面临一系列挑战和困难, 包括固体样品光散射问题, 反射模式收集样品光谱信号解析复杂; 固体样品介质与强光相互作用导致非线性光学效应问题; 固体样品中分子间相互作用导致激发态过程更复杂; 固体样品中界面和缺陷对激发态过程影响; 晶体相的激发态和瞬态中间体的电子结构的模拟等。因此本课题组利用超快光谱开展了有机固体光功能材料的激发态时间分辨探测与调控的探索工作, 揭示了激发态构效、电子结构与反应活性的内在关系, 1-7进而实现对激发态的调控, 为光功能材料设计提供理论指导和科学依据。

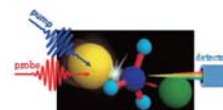


Fig. 1 Direct detection of excited states and transient species of molecule by pump-probe time-resolved spectroscopies

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## 参考文献

- Li, M. D.; Wong, N.; Zhu, R.; Wu, L.; Dai, S.; Su, T.; Chen, X. B.; Fang, W. H.; Yang, D.; Phillips, D. L. *J. Am. Chem. Soc.*, 2018, 140, 15957.
- Deng, Z.; Sun, S.; Zhou, M.; Huang, G.; Pang, J.; Dang, L.; Li, M. D. *J. Phys. Chem. Lett.*, 2019, 10, 6499.
- Huang, Q. Q.; Li, Y. Z.; Zheng, Z.; Jiang, X. M.; Sun, S.; Jiang, H. J.; Deng, W. H.; Wang, G.; Zhai, T. Y.; Li, M. D.; Xu, G. *CCS Chemistry*, 2019, 1, 655.
- Shan, S. S.; Pang, J.; Ni, S.; Zhang, G. H.; Xu, L.; Dang, L.; Li, M. D. *J. Phys. Chem. C*, 2020, 124, 17744.
- Luo, D.; Yang, S.; Zhang, Q.; Cha, L.; Dang, L.; Li, M. D. *J. Phys. Chem. Lett.* 2021, 12, 1838-1846.
- Pang, J.; Deng, Z.; Sun, S.; Huang, G.; Zhang, G.; Islam, A.; Dang, L.; Phillips, D. L.; Li, M. D. *J. Phys. Chem. Lett.*, 2021, 12, 41.
- Huang, G.; Li, J.; Deng, Z.; Li, J. H.; Sun, S.; Xu, L.; Dang, L.; Li, M. D. *J. Phys. Chem. Lett.* 2021, 12, 4306-4312. (Back cover)
- Chen, W. B.; Sun, S.; Huang, G.; Ni, S.; Xu, L.; Dang, L.; Phillips, D. L.; Li, M. D. *J. Phys. Chem. Lett.* 2021, 12, 5796-5801. (Front cover)

## 报告摘要

## 邀请报告

## New Phase Space Formulation of Quantum Dynamics for Nonadiabatic Systems

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We report recent progress on the phase space formulation of quantum mechanics with coordinate-momentum variables. We will focus on the phase space mapping theory for nonadiabatic systems where electronic degrees of freedom are treated as discrete variables and nuclear degrees of freedom as continuous variables. The topics include a unified framework for constructing the phase space mapping Hamiltonian, a general phase space formulation of quantum mechanics for nonadiabatic systems where a finite number of discrete electronic states are mapped onto constraint space and nuclear degrees of freedom are mapped onto infinite space, and an isomorphism between the mapping phase space approach for nonadiabatic systems and that for nonequilibrium electron transport processes. It is shown that the conventional zero-point-energy parameter should be interpreted as a special case of a commutator matrix in the comprehensive phase space mapping Hamiltonian for nonadiabatic systems. Our applications range from gas phase to condensed phase systems, which include the spin-boson model for condensed phase dissipative two-state systems, the three-state photo-dissociation models, the seven-state Fenna-Matthews-Olson monomer that appears in photosynthesis in green sulfur bacteria, strongly coupled optical cavity-molecular matter systems used to control and manipulate chemical and physical processes, singlet-fission systems, and so forth.

## References

- [1] J. Liu, *J. Chem. Phys.* 2016, 145: 204105
- [2] J. Liu, *J. Chem. Phys.* 2017, 146: 024110
- [3] X. He, J. Liu, *J. Chem. Phys.* 2019, 151: 024105
- [4] X. He; Z. Gong, B. Wu, J. Liu, *J. Phys. Chem. Lett.* 2021, 12, 2496–2501
- [5] X. He; B. Wu, Z. Gong, J. Liu, *J. Phys. Chem. A* 2021, 125, 6845–6863
- [6] J. Liu, X. He, B. Wu, *Acc. Chem. Res.* 2021, 54, 4215–4228
- [7] X. He, B. Wu, Y. Shang, B. Li, X. Cheng, *Wiley Interdiscip. Rev. Comput. Mol. Sci.* 2022, e1619 <https://doi.org/10.1002/wcms.1619>
- [8] X. He, B. Wu, T. Rivlin, J. Liu, E. Pollak, *J. Phys. Chem. Lett.* 2022, 13, 6966–6974

## 报告摘要

## 邀请报告

## Liquid-Vapor Surface Photoelectron Spectroscopy: a Test for Decoding Electronic Structure of Salted Water

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Mangy basic questions concerning ion solvation behavior at the simplest aqueous interface, namely the air or liquid vapor/ liquid water interface or, in other words, the open aqueous surface remain still unclear and unanswered. Similarly, little is known about the dynamical change of water hydrogen bonding near hydrophobic surfaces upon the addition of salt to liquid water. Thus, knowledge of the surface molecular geometric and electronic structures of aqueous solutions is a prerequisite to understanding these seemingly basic questions, many biological processes and technological applications, such as salt ion solvation, protein folding and interfacial catalysis.

Experimental techniques capable of accessing the details of surface molecular geometric and/or electronic structures and even molecular interactions at liquid aqueous interfaces with angstrom resolution have matured only recent years. These include primarily nonlinear optical techniques, such as vibrational sum-frequency generation (VSFG) and second harmonic generation (SHG) spectroscopies. Despite this impressive progresses, photoelectron spectroscopy (PES) has been verified to be an ideal tool to directly obtain molecular electronic structures and successfully applied in recent years to molecular spectroscopy and dynamics in the gas or solid systems. However, experimental investigations of the electronic structure of aqueous solutions have only recently become possible by using PES in combination with a liquid microjet technique. **Currently, we have succeeded in building the PES of liquids. Particularly, we have also succeeded in building a novel liquid-microjet photoelectron imaging (PEI) spectrometer [1].**

**Applications of liquid microjet PES to investigate electronic structure of liquid-vapor surface of salted water are given here.** The liquid PES and vapor PES are well characterized and identified. Our work demonstrates for the feasibility to make such a direct comparison between surface and bulk-solution electronic properties, suggesting liquid microjet PES is indeed most suited for measuring electronic structure of the solution surface or the bulk of solutions.

**Acknowledgements:** This work has the support of by the National Natural Science Foundation of China (No. 21327804).

## References

- [1] J. Long, Z. Qiu, J. Wei, D. Li, X. Song, B. Jin, B. Zhang\*, *Rev. Sci. Instrum.*, 92, 065108 (2021).



## 报告摘要

## 邀请报告

## The formation dynamics of o-benzyne in liquid phase

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The o-benzyne is a highly reactive intermediate which has been investigated for almost one century in organic chemistry. Although much structural and spectroscopic information of o-benzyne has been collected in gas or solid phase at low temperature, the direct spectroscopic observation of its formation dynamics is still missing at least in the liquid phase. In this talk, I will report our recent work on ultrafast formation dynamics of o-benzyne from two important precursors in liquid phase. Upon the UV optical excitation, while the subsequent photochemistry and photophysics is observed by using fs-TA spectroscopy in both the UV/Vis and mIR regime.

(1) The ultrafast photoinduced behaviour of benzocyclobutenedione (BCBD) in dichloromethane solution is investigated upon 300 nm excitation. In addition to the ultrafast electronic deactivation in several ps, three photochemical channels (ring-opening, carbene formation and decay, de-CO and rearrangement leading to o-benzyne) with multiple intermediates have been identified, revealing the complicated dynamics on a time scale ranging from hundreds of fs to several ns.

(2) The o-benzyne derivatives are believed to be the initial products of the so-called hexadehydro-Diels-Alder (HDDA) reaction. We therefore investigated the photoinduced dynamics of a bis-diyne compound upon UV excitation in liquid phase. For identification of the formed o-benzyne species, we employed two intermolecular trapping strategies, i.e. self-trapping and trapping by perylene. Reconstruction of the spectrum of trapping products provide a convincing picture for o-benzyne formation in solution as primary product of photochemical HDDA reactions.

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## References

- [1] X. Ma, T. Brixner, etc., Phys. Chem. Chem. Phys., 20, 15434-15444 (2018).  
[2] X. Ma, T. Brixner, etc., Chem. Sci., 11, 9198-9208 (2020).

## 报告摘要

## 邀请报告

## 锂电池的界面结构与离子脱嵌化学动力学

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摘要: 锂电池的界面结构与离子脱嵌动力学研究: (a) 建立原子尺度原位界面结构化学与电化学协同研究方法, 探索了锂电池正极的界面结构与电化学窗口相关性以及碳负极界面电化学重构形成固态电解质膜 (SEI膜) vs 离子脱嵌机理; (b) 发展中子和同步辐射X射线联合测量溶液和晶体的局域/长程结构, 原位检测发现锂电池正极的过渡金属自旋电子与微波的共振作用使得材料几分钟升温到近千度和微波“靶向”驱动锂离子快速嵌入制备锂电池层状材料的机理; (c) 探索了锂电池电解液从稀到超浓的溶液结构, 发现超浓溶液电化学窗口拓展是因为界面离子脱嵌动力学能垒提升而不是溶液结构的热力学贡献; (d) 系统探索和总结了锂电池界面结构/重构 vs 电化学, 发现磷酸铁锂在水电解质体系形成Junas界面, 使得锂离子脱溶剂化嵌入晶格能垒极低, 实现锂电池几秒完成充放电。

## 参考文献

- F. Pan\* et al (1) Structural origin for the high voltage instability of lithium cobalt oxide, Nature Nanotech (2021), DOI: 10.1038/s41565-021-00855-x; (2) In situ quantification of interphasial chemistry in Li-ion battery, Nature Nanotech., (2019) 14(1) 50; (3) Ultrafast solid-liquid intercalation enabled by targeted microwave energy delivery, Science Adv (2020), 6 (51) eabd9472; (4) Understanding Thermodynamic and Kinetic Contributions in Expanding the Stability Window of Aqueous Electrolytes, Chem, (2018), 4(12) 1-11; (5) Harnessing the surface structure to enable high-performance cathode materials for lithium-ion batteries", Chem. Soc. Rev. (TUTORIAL REVIEW) (2020) 49, 4667, (6) "Origin of structural degradation in Li-rich layered oxide cathode", Nature, 2022, 606, 305

## 报告摘要

## 邀请报告

Fermi-phase-induced interference in the reaction of Cl with vibrationally excited CH<sub>2</sub>DHuilin Pan<sup>1,2</sup>, and Kopin Liu<sup>2,3</sup><sup>1</sup>Department of Chemistry, Southern University of Science and Technology, Shenzhen 518055<sup>2</sup>Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617<sup>3</sup>State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Dalian 116023

Mode selectivity is a well-established concept in chemical dynamics. Unlike a diatom, a polyatomic molecule possesses multiple vibrational modes. Different vibrational motions can have vastly distinct capacities of promoting or hindering reactivities. Up to now, the key idea underlying mode selectivity is based on the amplitudes of vibrational motions [1], which can often be understood in terms of a classical oscillator. However, there are other types of molecular vibrations that are intrinsically quantal in nature and thus cannot be visualized in this way. One example is Fermi-coupled vibration [2].

Here, I will present our recent study to address the effects of the Fermi phase on chemical reactivity [3]. In CH<sub>2</sub>D, the strong Fermi interaction between  $\nu_1 = 1$  (or  $11_1$ ), CH<sub>2</sub> symmetric-stretching mode) and  $\nu_5 = 2$  (or  $15_2$ ), the CH<sub>2</sub> degenerate deformation mode) results in two eigenstates  $\nu_1$ -I and  $\nu_1$ -II, which are the superposition states of  $|11_1\rangle$  and  $|15_2\rangle$  with comparable yet opposite-signed mixing coefficients [4]. Physically,  $\nu_1$ -I and  $\nu_1$ -II may be regarded as synchronized vibrational motions with similar amplitudes, but opposite phases. Experimentally, we found that exciting  $\nu_1$ -I and  $\nu_1$ -II of CH<sub>2</sub>D greatly accelerated the reaction with Cl [3]. However, the reactivity ratio of  $\nu_1$ -I/ $\nu_1$ -II deviated significantly from that permitted by the conventional reactivity-borrowing framework [5]. This discrepancy can only be explained when the scattering interferences induced by the Fermi phase are explicitly considered, which we coined the Fermi-phase-induced interference. This work gives a clear demonstration of quantum-phase control of bimolecular reactions and expands the concept of vibrational control of chemical reactivity into quantum regime. The method proposed here is general and should be applicable to any chemical processes involving superposition quantum states.

## References

- [1] H. Guo, B. Jiang, *Acc. Chem. Res.*, 47, 3679–3685 (2014).
- [2] G. Herzberg, *Molecular Spectra and Molecular Structure, Vol. II: Infrared and Raman Spectra of Polyatomic Molecules* (Van Nostrand-Reinhold, 1945).
- [3] H. Pan, K. Liu, *Nat. Chem.*, 14, 545-549 (2022).
- [4] X. G. Wang, E. L. III Silbert, *J. Chem. Phys.*, 111, 4510–4522 (1999).
- [5] R. Ellerbrock, U. Manthe, *J. Chem. Phys.*, 147, 241104 (2017).

## 报告摘要

## 邀请报告

## Combustion Diagnostics and Its Applications in Reacting Flow

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Reliable and predictable combustion model can help us to understand the combustion process deeply, and potentially help us to design higher-performance engines, increase combustion efficiency and reduce harmful emissions. However, the development of combustion model is badly relied on the advances of experimental and diagnostic methods.

In this talk, photoionization mass spectrometry and laser spectroscopy/imaging will be introduced for applications in study of reaction kinetics and flow dynamics, respectively. Benefiting from the novel design and the upgraded instruments located at Hefei Light Source, a lot of "new" reactive species can be unambiguously detected, i.e., H, O, OH, and hydroperoxides [1]. Furthermore, the techniques can be applied in the detection of gas-phase products of heterogeneous reactions including catalysis reaction, biomass pyrolysis etc. [2-4].

Recently, we utilized high-repetition (100 kHz) burst laser and diode laser to develop various novel diagnostics for simultaneous measurement of flow field, temperature and species in swirling flame and turbulent jet flame. The temporal-spatial-resolved measurement of the flow and flame structures and their evolutions enabled us to understand the vortex-flame dynamics related to combustion instability problems [5-6]. Furthermore, it provided us with a physical picture of how thermal acoustic instabilities can be suppressed based on vortex tuning using various control strategies [7].

## References

- [1] Z. Zhou, X. Du, et al., *Journal of Synchrotron Radiation*, 23 1035 (2016).
- [2] F. Jiao, J. Li, et al., *Science*, 351 1065 (2016).
- [3] W. Wen, S. Yu, et al., *Angew. Chem. Int. Ed.*, 59 4873 (2020).
- [4] J. Hu, L. Yu, et al., *Nature Catalysis*, 4 242 (2021).
- [5] G. Wang, X. Liu, et al., *Proc. Combust. Inst.*, 38 6183-6191 (2021).
- [6] X. Xia, C. Fu, et al., *Proc. Combust. Inst.*, 38 2067-2074 (2021).
- [7] L. Xu, J. Zhen, et al., *Proc. Combust. Inst.*, 38 6095-6103 (2021).



## 报告摘要

## 邀请报告

## Understanding Carrier Dynamics in Quasi-2D Hybrid Halide Perovskite

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The 2D Ruddlesden-Popper (RP) perovskite is considered as one of the most promising evolutions in optoelectronic materials field. Unique stability and excellent optoelectronic properties make it a research hotspot. However, the spatial phase distribution and the band alignment of the quasi-2D perovskite is still under debate, which leads to more puzzling carrier dynamics. Here, we used the highly sensitive transient absorption spectroscopy to investigate the carrier dynamics of  $(\text{BA})_n(\text{MA})_{n-1}\text{PbI}_{3n-1}$  quasi-2D RP perovskite thin film, nominally prepared as  $n=4$ . The carrier density-dependence of both electron and hole transfer dynamics was observed between multiple phases with small  $n$  ( $n=3, 4$  and  $5$ ) and  $n=\infty$  phases. From their genuine dynamics under low carrier density in the linear response range, three ultrafast processes of the electron and hole transfers were clearly resolved, lasting hundreds fs to several ps, tens to hundreds ps and hundreds ps to several ns, respectively. They were attributed to lateral epitaxial, partial epitaxial and vertical van der Waals heterostructures between small  $n$  and  $n=\infty$  phases. Further, we can determine their type II band alignment structures. These results provide deep insights into an accurate intrinsic photo-physics of 2D perovskites with direct implications for photovoltaic and optoelectronic material improvements and applications.

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[2] F. L. Author, H.-G. Test, book title (publishing company, place, year).

## 报告摘要

## 邀请报告

## New developments of the hierarchical equations of motion method: Tensor network implementation, phase space formulation, and equilibrium correlation functions

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The non-perturbative hierarchical equations of motion (HEOM) method has recently developed into an important tool to simulate quantum dynamics in condensed phase. I will present some recent progresses in our group on the methodology developments: (1) New algorithms that can efficiently treat complex system-bath interactions based on the tensor network representation. The matrix product state (MPS) and tree tensor network (TTN) methods now allow simulation of HEOM with  $10^2$ - $10^3$  effective modes. (2) Recent works have shown that there are numerical stability issues of the HEOM with discrete harmonic oscillator modes and multiple Brownian oscillator spectral density. By writing the HEOM into phase space equations of motion, we are able to resolve this problem by deriving an equivalent set of equations in a new set of basis set. (3) Imaginary time HEOM to calculate the equilibrium of the total system and equilibrium correlation functions. In combination with the phase space formulation, we are also able to extend our previous mixed quantum-classical non-adiabatic reaction rate theory to full quantum regime.

**Keywords:** hierarchical equations of motion, matrix product state, tree tensor network, numerical stability, charge and energy transfer

## References

- [1] Q. Shi, Y. Xu, Y.-M. Yan, and M. Xu, *J. Chem. Phys.* 148, 174102 (2018).
- [2] Y.-M. Yan, T. Xing, and Q. Shi, *J. Chem. Phys.* 153, 214109 (2020).
- [3] Y.-M. Yan, M. Xu, T.-C. Li, and Q. Shi, *J. Chem. Phys.* 154, 194104 (2021).
- [4] T.-C. Li, Y.-M. Yan, and Q. Shi, *J. Chem. Phys.* 156, 064107 (2022).
- [5] T. Xing, T.-C. Li, Y.-M. Yan, S.-M. Bai, and Q. Shi, *J. Chem. Phys.* 156, 244102 (2022).
- [6] T. Xing, T.-C. Li, Y. Liu, and Q. Shi, *Chin. J. Chem. Phys.*, in press 2022.

## 报告摘要

## 邀请报告

## 电子与气液界面的碰撞反应

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气液界面的微观结构和化学反应仍然是当前物理化学研究的难点, 但是其具有广泛而重要的研究意义。由于气液界面在分子密度、空间分布方面与气相(自由气体)和液相存在很大差异, 因此, 在这样一个非均相环境中发生的化学反应会具有显著不同的反应机制。

为此, 我们利用微喷射流(microjet)产生液束(直径25微米)技术, 建立了一套新型的质谱方法: 时间延迟质谱(time-delayed mass spectrometry, TDMS)。利用此方法, 我们先后成功观测到了气液界面的分子取向、原位分子团簇等微观结构信息[1-3]。最近, 我们观测到了气液界面处的电子诱导化学反应以及电子黏附解离, 这些过程的动力学特征明显不同于气相、固相的相关过程[4, 5]。我们受邀评述了以上进展[6]。



图 1: TDMS装置与部分实验结果

## 参考文献

- [1] Chen, L.; et al. *Rev. Sci. Instrum.* 2018, 89: 103102.
- [2] Chen, Z. et al. *J. Phys. Chem. Lett.* 2020, 11: 7510.
- [3] Li, Z.; et al. *Chin. J. Chem. Phys.* 2021, 34: 43.
- [4] Li, Z.; et al. *J. Phys. Chem. Lett.* 2022, 13: 5220.
- [5] Chen, Z.; et al. (to be submitted).
- [6] Chen, Z.; Li, Z.; Hu, J.; Tian, S.X. *Acc. Chem. Res.* (submitted).

## 报告摘要

## 邀请报告

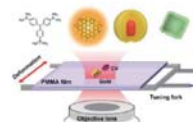
## Single molecule spectroscopy for sensing and photophysics

Mingcai Xie, Sushu Wan, Zhihong Wei, Yu Du, Weiqing Yang and Yuxi Tian\*

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Single molecule spectroscopy provides us with the opportunity to investigate the fundamental principles at the single molecule level. Unique optical properties of individual molecules and particles have been reported. In addition, SMS also allows us to expect functional devices based on a single molecule. Recently, we successfully achieved ultrasensitive detection of weak acoustic waves by detecting fluorescence from a single molecule. We also investigated fundamental photophysical processes in novel optoelectric materials at the individual particle level, including organometal halide perovskite, quantum dots and carbon dots. In this talk, I will briefly present our recent work on these systems.



**Acknowledgements:** This work was supported by the National Natural Science Foundation of China (NSFC no. 22073046 and 62011530133). This work was also supported by State Key Laboratory of Analytical Chemistry for Life Science (SKLACL2217) and the Fundamental Research Funds for the Central Universities (020514380256 and 020514380278).

## References

1. Xie, M. et al. *Nat. Commun.* 13, 3330 (2022).
2. Wang, B. et al. *Light Sci. Appl.* 11, 172 (2022).
3. Xie, M. et al. *J. Phys. Chem. Lett.* 13, 2371-2378 (2022).
4. Wei, Z. et al. *Chinese Chem. Lett.* 33, 751-756 (2022).
5. Du, Y. et al. *J. Phys. Chem. Lett.* 12, 7106-7112 (2021).
6. Du, Y. et al. *J. Phys. Chem. Lett.* 12, 773-780 (2021).

## 报告摘要

## 邀请报告

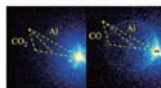
## Imaging stereodynamics in metal atom collisions

Yujie Ma, Fangfang Li, Dong Yan, Ang Xu, Jiaying Liu, Fengyan Wang\*

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Stereodynamics in atom-molecular collisions are closely related to efficient energy transfer between collision partners during interactions. The single-collision dynamics between metal atoms and small molecules ( $O_2$ ,  $CO$ ,  $CO_2$ ,  $CH_4$ , etc.) was investigated by using the laser-ablation crossed molecular beam and time-sliced ion velocity imaging setup. The velocity and angular distributions of scattering reactants and products provide detailed stereo dynamic information on elastic, inelastic and reactive collisions. Some interesting results are observed. (1) The nonadiabatic electronic transitions of metal atoms in inelastic collision were observed at small impact parameters. In the collision of Y atoms with rare gas atoms, the spin-orbit splitting excited  $Y(^2D_{5/2})$  atoms from the inelastic scattering show the backward angular distribution, indicating that the electronic excitation occurs at small impact parameters. (2) The elastic collisions of Al atoms with  $O_2$ ,  $CO$  and  $CO_2$  molecules exhibit different scattering angular distributions, indicating different long-range attractive forces at large impact parameters. (3) The bending excitation of  $CO_2$  inhibits the reaction with Al atoms in a wide range of collision energies. With the heated valve for  $CO_2$ , the AlO products were exclusively generated by the reactions of ground  $CO_2$  with Al atoms. In the elastic collision with  $CO_2$  molecules, the sharp forward scattering of Al atoms suggests that the long-range attractive force is weak. The reactive and elastic collisions suggest the collinear collision geometry for the reaction with an early barrier.

Figure 1: Scattering of Al atoms from collisions with  $CO_2$  and  $CO$  molecules.

## Acknowledgements:

The work was supported by the National Natural Science Foundation of China (No.21327901 and No.22073019), the Shanghai Key Laboratory Foundation of Molecular Catalysis and Innovative Materials, and the Program for Professor of Special Appointment (Eastern Scholar) at Shanghai Institutions of Higher Learning.

## References

[1] Xu, A.; Ma, Y.; Yan, D.; Li, F.; Liu, J.; Wang, F. *Chin. J. Chem. Phys.* 34, 61(2021). [2] Li, F.; Dong, C.; Chen, J.; Liu, J.; Wang, F.; Xu, X. *Chem. Sci.* 9, 488(2018).

## 报告摘要

## 邀请报告

## Understanding Protein Chirality and Charged Interface Through Surface Nonlinear Spectroscopy

Hong-fei Wang<sup>1</sup>\*, Xiao-Hua Hu<sup>2</sup>, and Hui Wang<sup>2</sup><sup>1</sup>School of Sciences, Westlake University, 18 ShiLongShan Road, Yunxi Town, Westlake District, Hangzhou, Zhejiang Province, 310024<sup>2</sup>Department of Chemistry, Fudan University, 220 Handan Road, Yangpu District, Shanghai 200433

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Using the newly developed phase-resolved chiral sum-frequency generation vibrational spectroscopy (PR-cSFG-VS), we found that the chirality of the N-H group in folded peptide was governed by the C-H chirality of the amino-acids in the peptide. This provides a direct handle to probe protein folding processes and to understand protein chirality. A theoretical formulation on the electric field induced (EFI) nonlinear optical responses from the charged interfaces was developed to describe the existing water/silica interface data in EFI second harmonic generation (EFI-SHG) data. These advances provide new answers and tools for future applications of surface nonlinear spectroscopy to problems in biological and energetic surface and interfaces.

**Key Words:** Protein Chirality, PR-cSFG-VS, Charged Interface, EFI-SHG

## Acknowledgements:

This work has the support of the National Natural Science Foundation of China (NSFC Grant No. 21727802), the Westlake University and the Westlake Education Foundation.

## References

[1] Xiao-Hua Hu, Li Fu, Jian Hou, Yue-Ning Zhang, Zhen Zhang, and Hong-Fei Wang\*, N-H Chirality in Folded Peptide LK7 $\beta$  Is Governed by the C-H Chirality, *J. Phys. Chem. Letts.*, 11, 1282-1290-2020. [2] Perets, Ethan A.; Konstantinovsky, Daniel; Fu, Li; Chen, Jiantao; Wang, Hong-Fei; Hammes-Schiffer, Sharon; Yan, Elsa C. Y., Mirror-image antiparallel beta-sheets organize water molecules into superstructures of opposite chirality, *Proc. Nat. Acad. Sci. U.S.A.*, 117 (52) 32902-32909, 2020. [3] Hui Wang, Xiao-Hua Hu, and Hong-Fei Wang\*, Charge-Induced  $\chi^{(3)}$  Susceptibility in Interfacial Nonlinear Optical Spectroscopy Beyond the Bulk Aqueous Contributions: The Case for Silica/Water Interface, *J. Phys. Chem. C* 125, 47, 26208-26215, 2021. [4] Xiao-Hua Hu, Feng Wei, Hui Wang, and Hong-Fei Wang\*, -Quartz Crystal as Absolute Intensity and Phase Standard in Sum-Frequency Generation Vibrational Spectroscopy, *J. Phys. Chem. C.*, 123, 15071-15086, 2019.

## 报告摘要 邀请报告

## Quantum state resolved reactive scattering experiments using the near threshold ionization method

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Accurate measurements of product state-resolved angular distributions are central to the studies of chemical reaction dynamics[1]. By using the near threshold ionization detection method, together with the time sliced velocity map ion imaging technique, high resolution state-to-state differential cross sections have been acquired for the H+HD, F+HD and N+HD reactions. These high-resolution experiments have played an important role in understanding quantum dynamics phenomenon in elementary chemical reactions.

**Acknowledgements:**

This work was supported by the National Key R&D Program of China, (Grant No. 2016YFF0200500), the National Natural Science Foundation of China (Grant No. 22125302) and Chinese Academy of Sciences (grant no. XDB 17010000).

**References**

[1] Xingan Wang and Xueming Yang, Science, 374, 938 (2021)

## 报告摘要 邀请报告

## Ultrafast extreme ultraviolet photoemission electron microscopy based on gaseous high-order harmonics

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Femtosecond laser has ultra-short pulse duration and ultra-high peak intensity. Its interaction with gaseous atoms and molecules is an extremely non-linear process and leads to some well-known strong field phenomena. The study on the interaction between intense femtosecond laser and atom / molecule provides novel schemes for generating tabletop advanced electron beam and light source, which greatly enrich the research tools of material science. We have set up an advanced experimental platform and studied the mechanism of femtosecond laser interacting with atoms and molecules [1-3]. In this talk, we report our newly built ultrafast extreme ultraviolet photoemission electron microscopy. High-order harmonics with high repetition rate and high flux are generated by the interaction of 800-nm femtosecond laser with noble gases in the hollow core fiber. A single order harmonic is selected out and combined with photoemission electron microscope. This ultrafast extreme ultraviolet photoemission electron microscopy provides an advanced tool for studying electron dynamics covering the full Brillouin zone of solid materials and micro-nano structures with ultrahigh time, space and energy resolution [4]. Finally, we demonstrate the characterization and manipulation of photoelectron emission from plasmonic nanostructures induced by strong femtosecond laser by using this powerful microscope.

**Acknowledgements:** This work has the support of National Key R&D Program of China (No. 2018YFA0306302) and the National Natural Science Foundation of China (Nos. 11625414, 11527901).

**References**

- [1] W. Zheng, Z. Miao, L. Zhang, Y. Wang, C. Dai, A. Zhang, Q. Gong, C. Wu. J. Phys. Chem. Lett 10, 6598 (2019).  
 [2] W. Zheng, Z. Miao, C. Dai, Y. Wang, Y. Liu, Q. Gong, C. Wu. J. Phys. Chem. Lett 11, 7702 (2020).  
 [3] P. Ge, Y. Fang, Z. Guo, X. Ma, X. Yu, M. Han, C. Wu, Q. Gong, Y. Liu, Phys. Rev. Lett., 126, 223001 (2021)  
 [4] W. Zheng, P. Jiang, L. Zhang, Y. Wang, Q. Sun, Y. Liu, Q. Gong, C. Wu, Rev. Sci. Instrum. 92, 043709 (2021).



## 报告摘要

## 邀请报告

## Ultrafast dynamics of molecules in superfluid helium nanodroplets

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Superfluid helium ( $^4\text{He}$ ) nanodroplets with an extremely cold environment at 0.37 K and a broad transparent spectral range are ideal nanoreactors for light-induced physical and chemical reactions of the embedded molecules. Most information of the in-droplet molecules is obtained from the spectroscopy measurements, although the dynamics are the key for one to understand and further control the chemical reactions. Here, by measuring the electrons and ions ejected from an in-droplet molecule in coincidence, as illustrated in Fig.1, we explore ultrafast dynamics of in-droplet molecules driven by femtosecond laser pulses [1].

We experimentally observed femtosecond laser pulse induced field-free molecular alignment dynamics of  $\text{D}_2$  inside He droplets. Our measurements show that for at least 100 ps, equivalent to  $> 500$  rotational periods,  $\text{D}_2$  molecules in He droplets rotate as if they were isolated gas-phase particles. This behavior is strikingly different from the in-droplet rotation of all other molecules studied. Our observations show that the  $\text{D}_2$  molecules inside helium nanodroplets essentially rotate as free  $\text{D}_2$  molecules. Furthermore, we experimentally investigated the above-threshold multiphoton ionization of  $\text{H}_2$  embedded in a superfluid helium nanodroplet. We find that the low-vibrationally excited in-droplet  $\text{H}_2^+$  is promoted to dissociate, while for the isolated gas-phase case only high-vibrationally excited  $\text{H}_2^+$  can dissociate. Our results are significant for understanding and further steering the light-induced molecular dynamics in helium nanodroplets.

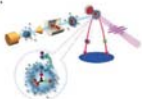


Figure 1: The schematic illustration of the COLTRIMS setup for investigation of ultrafast dynamics of the in-droplet molecules.

## References

[1] J. Qiang et al, Phys. Rev. Lett. 128, 243201 (2022); L. Zhou et al, Phys. Rev. Lett. (2022), in revision.

## 报告摘要

## 邀请报告

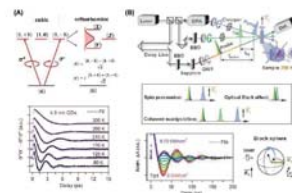
## 胶体量子点自旋相干动力学

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胶体量子点与外延生长量子点相比具有制备成本低、物理化学性质易调谐等优势, 但在量子光学、量子信息等领域的应用面临巨大挑战。主要原因在于胶体量子点的激子和载流子自旋相干寿命极短。我们基于瞬态圆二色谱技术对新兴的铅卤钙钛矿胶体量子点自旋动力学开展了系统的研究。首先, 我们在限域较强的CsPbI<sub>3</sub>量子点中观测到了系综层面、零磁场下的激子自旋量子拍频, 对应于明态激子的各向异性交换劈裂[1], 劈裂能高达1.6meV, 且可以通过温度进行调节。变温结构表征表明这种温度调谐性来源于CsPbI<sub>3</sub>钙钛矿晶格对称性的温度依赖: 温度越低, 晶格扭曲越强烈, 对称破缺越明显, 相应的FSS越大, 拍频的频率越大。由于激子自旋的相干寿命仍然仅有几个ps, 我们进而研究单载流子态的自旋相干[2]。我们利用光致超快电子转移在量子点中留下自旋极化的单空穴态, 在室温下达到百ps量级。在此基础上, 利用超快自旋操控技术, 通过光学斯塔克效应产生预磁场率先实现了室温下量子点自旋的相干操控。



## References

[1] Yaoyao Han, Wenfei Liang, Xuyang Lin, Yulu Li, Fengke Sun, Fan Zhang, Peter C. Sercel, Kaifeng Wu. arXiv:2206.13716 (Nat. Mater. in press)

[2] Xuyang Lin, Yaoyao Han, Jingyi Zhu, Kaifeng Wu. Under review



报告摘要

邀请报告

Optical strategies towards interlayer coupling and functionalities at two-dimensional interfaces

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Benefiting from the great success of the structure-property relationship study on single nanomaterial units, the concept of bottom-up assembly provides rich inspiration for people to design and construct new materials and devices. Interface interactions unusually play a critical role in such cases and have brought about various previously inaccessible interesting physical properties, yet they are mysterious and hard to be fully deciphered. Herein, we will start from the mechanical coupling behavior between interlayer phonons and plasmonic metals, noted as mechano-Raman scattering (MRS). The unique thermal-noise-free feature of MRS, as well as the capacity towards characterization of global crystal fine structure and hidden interfaces will be demonstrated in sequence. Furthermore, we will focus on the interfaces of the simplest two-dimensional (2D) bilayer heterostructure. Their unique interfacial processes involving excitons<sup>1</sup>, carriers<sup>2,3</sup>, chemical reactions at the 2D heterogeneous interfaces with different coupling distances, as well as the related sensing applications will be presented and discussed, respectively. Just like organic chemists who use atoms to build molecules with different structures and activities, our study will provide insights for the design and development of low-dimensional quantum materials and devices with conceptually-new functionalities.

**Acknowledgements:** This work has the support of the National Natural Science Foundation of China (21873048; 22173044), the National Key R&D Program of China (2020YFA0406104) and Excellent Youth Fund of Jiangsu Province (BK20220121).

References

- [1] Jiang C.Y. #, Xu W.G. #, et al., Nature Communications, 9, 753 (2018).
- [2] Xu W.G., Liu W.W., et al., Nature, 541, 62 (2017).
- [3] Li H., Li H.L., et al., Nano Letters, 21, 6773 (2021).

报告摘要

邀请报告

Anomalous Vibrational Spectra: The Symmetry Dilemma of Doubly Hybrid Density Functionals

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In electronic structure theory, when an approximate wavefunction tends to artifactually break the symmetry of the exact Hamiltonian, the corresponding method is referred to as having a "symmetry dilemma" problem<sup>1</sup>. When this symmetry dilemma tends to happen, property predictions such as dipole moment, static polarizability and vibrational frequency can become totally unreliable, e.g., showing a qualitatively wrong polarizability with a negative sign and an unphysical frequency that is over 300% larger.

Doubly hybrid (DH<sup>2,3</sup>) functionals belong to a new generation of density functional theory (DFT) methods. Especially, with the development of the second order analytic derivatives, the DH functionals were shown to be able to yield excellent vibrational frequency predictions comparable to the gold standard method, i.e., CCSD(T), in the wavefunction theory.<sup>4,5</sup> In this talk, we present a systematic report on the reliability of the DH functionals for several violable cases. Almost all the commonly used B2PLYP type (bDH<sup>2</sup>) functionals are shown to have a severe "symmetry dilemma" problem and yield dramatically unreliable molecular properties at the equilibrium geometry.<sup>6,7</sup> It is remarkable that the XYG3 type (xDH<sup>3</sup>) functionals show a good capability to resist the artifactual symmetry breaking and yield reliable molecular properties when the same critical cases are calculated.<sup>7</sup> The insights gained in this work are of great significance not only for DFT applications, but also for the development of an ever better DFT functional.

**Acknowledgements:** We appreciate the support from National Natural Science Foundation of China (Grant 21688102).

References

- [1] P. O. Löwdin, Rev. Mod. Phys., 35, 496 (1963).
- [2] S. Grimme, J. Chem. Phys., 124, 034108 (2006).
- [3] Y. Zhang, X. Xu, W. A. Goddard III, Proc. Natl. Acad. Sci. USA., 106, 4963 (2009).
- [4] M. Biczysko, P. Panek, G. Scalmani, J. Bloino, V. Barone, J. Chem. Theory Comput. 6, 2115 (2010).
- [5] Y. Gu, Z. Zhu, X. Xu, J. Chem. Theory Comput. 17, 4860 (2021).
- [6] J. M. Simmie, K. P. Somers, J. Phys. Chem. A 124, 6899 (2020).
- [7] Y. Gu, X. Xu, J. Chem. Theory Comput. 17, 7745 (2021).
- [8] F. L. Author, H.-G. Test, book title (publishing company, place, year).

## 报告摘要

## 邀请报告

## Making molecular movies for gaseous molecules with mega-electron-volt ultrafast electron diffraction

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Since the birth of femtosecond lasers in 1980s, ultrafast laser spectroscopy has been serving as the major workhorse for the advancement of ultrafast molecular science. Nevertheless, given that spectroscopy is an indirect probe for molecular structure, a direct technique for probing molecular structural evolution under femtosecond timescales, i.e. making molecular movies, is still lacking.

Making molecular movies requires the combination of sub-Å spatial resolution and femtosecond time resolution. For gaseous molecules, such an extreme spatiotemporal resolution was achieved in 2016 at SLAC National Lab using mega-electron-volt ultrafast electron diffraction (MeV-UED) [1,2]. Since this breakthrough, a series of nonadiabatic molecular movies have been recorded at SLAC [3-5].

In this presentation, I will introduce several latest achievements in molecular moviemaking using MeV-UED in the gas phase. We have resolved 1. Nuclear wavepacket splitting at conical intersections in CF<sub>4</sub> Rydberg state [3]; 2. Cyclohexadiene ground state dynamics after electrocyclic ring-opening [4]; 3. Nuclear and electronic degrees of freedom during pyridine internal conversion process [5].

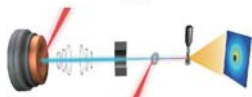


Figure 1: Mega-electron-volt ultrafast electron diffraction setup

## Acknowledgements:

This work has the support of U.S. Department of Energy.

## References

- [1] J. Yang, etc., Phys. Rev. Lett., 117, 153002 (2016).
- [2] J. Yang, etc., Nat. Commun., 7, 11232 (2016).
- [3] J. Yang, etc. Science, 361, 64-67 (2018)
- [4] T. Wolf, etc. Nat. Chem., 11, 504-509 (2019)
- [5] J. Yang, etc. Science, 368, 885-889 (2020)

## 报告摘要

## 邀请报告

A Ten-Dimensional Quantum Dynamics Study of the H + CH<sub>3</sub>D ReactionMingjuan Yang<sup>1</sup>, Tong Cheng<sup>2</sup>, Rui Zheng<sup>2</sup>,  
Hongwei Song<sup>1</sup> and Minghui Yang<sup>1\*</sup><sup>1</sup>Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences, Wuhan 430071, China<sup>2</sup>School of Mathematics and Information Science, North China University of Water Resources and Electric Power, Zhengzhou 450011, China

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The H + CH<sub>3</sub>D → H<sub>2</sub> + CH<sub>3</sub>D and H + CH<sub>3</sub>D → HD + CH<sub>3</sub> reactions were studied using a recently developed ten-dimensional time-dependent wave packet method [1]. The reaction dynamics are studied for the reactant CH<sub>3</sub>D initially from the ground state, the CH<sub>3</sub> symmetry and asymmetry stretching excitation, the CD stretching excitation and the fundamental and the first overtone of the CH<sub>3</sub> bending mode. For the H + CH<sub>3</sub>D → H<sub>2</sub> + CH<sub>3</sub>D reaction, the calculated reaction probabilities show that exciting either of the CH<sub>3</sub> stretching modes enhances the reactivity in the collision energy range below 1.0 eV, while the CD stretching excitation does not obviously prompt the reaction. Fundamental CH<sub>3</sub> bending excitation has nearly no effect on promoting reactivity. However, a significant enhancement is observed for the first overtone excitation of the CH<sub>3</sub> bending mode, resulting from the Fermi resonance between the fundamental state of the CH<sub>3</sub> symmetry stretching mode and the first overtone state of the CH<sub>3</sub> bending mode. While for the H + CH<sub>3</sub>D → HD + CH<sub>3</sub> reaction, the CD stretching excitation significantly prompts the reaction and both the CH<sub>3</sub> symmetric stretching and the first overtone excitation of the CH<sub>3</sub> bending mode slightly enhance the reactivity.

**Acknowledgements:** This work has the support of by the National Natural Science Foundation of China (Grant nos. 21973108 to MY, 21973109 to HS).

## References

- [1] R. Liu, H. Song, J. Qi and M. Yang, J. Chem. Phys. 153, 224119 (2020)

## 报告摘要

## 邀请报告

## Developing Laser Cooling System for Cold and Controlled Chemical Reactions Dynamics

Xiao Yue, Liu Lan, Xie Yurun, Liu Heyang, Wang Yuzhao, Li Jiayue, Peng Yongxu, Wen Liping, Yang Tiangang\*, Yang Xueming

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Reactions between molecules and ions at low temperature are of significant importance in both fundamental chemistry as well as in interstellar medium. Control over reactant translational and internal energies are necessary for addressing these reactions experimentally in detail. Recently, we have developed a new platform for quantum-state-resolved ion-molecule chemistry by utilizing a combination of cryogenic buffer gas cooling and laser-cooled ion sympathetic cooling in a radio frequency ion trap. In this talk, I will report the progress of this system and provide our recent results on the reaction dynamics of trapped, cooled ions and quantum-state-controlled molecules. ADDIN EN.CITE (1, 2) .

## References

- [1]. T. Yang et al., Optical control of reactions between water and laser-cooled Be<sup>+</sup> ions. *J Phys Chem Lett* 9, 3555-3560 (2018).
- [2]. T. Yang et al., Isomer-specific kinetics of the C<sup>+</sup>+ H<sub>2</sub>O reaction at the temperature of interstellar clouds. *Science Advances* 7, eabe4080 (2021).

## 报告摘要

## 邀请报告

## 小分子极紫外光化学研究

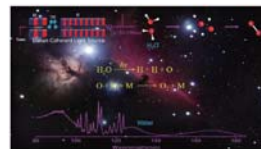
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分子光化学动力学研究在过去几十年取得了很大进展, 几乎所有小分子在紫外波段(200-400nm)的光化学都有研究报道, 而在极紫外波段(50-150nm), 受限于高亮度可调谐的极紫外光源的缺乏和实验探测的困难, 分子在这一波段的研究国内外都比较稀少。而恰恰宇宙诞生早期最重要的一些分子, 比如H<sub>2</sub>O, CO<sub>2</sub>, CH<sub>4</sub>等分子的光化学都位于极紫外区, 对于这些分子的光化学过程应该怎么去研究呢? 过去三年来, 我们利用大连极紫外自由电子激光和桌面激光器产生的极紫外光源, 系统的研究了水分子和硫化氢分子在极紫外区域的光化学反应过程, 并探讨了这些过程在星际空间的影响。



图一、大连极紫外自由电子激光研究水分子三体解离以及其对行星早期大气产氧的意义。

关键词: 分子光化学; 极紫外光; 大连相干光源

## 参考文献

- [1] Y. Chang, et al., K. J. Yuan\*, and X. M. Yang\*, *Nat. Commun.* 10, 1025 (2019).
- [2] J. M. Zhou, et al., M. N. R. Ashfold\*, K. J. Yuan\*, X. M. Yang\*, *Nat. Commun.* 11, 1547 (2020).
- [3] Y. Chang, et al., M. N. R. Ashfold, K. J. Yuan\*, X. M. Yang\*, *Nat. Commun.* 12, 2476, (2021). (Featured Article)
- [4] Z. J. Luo, Y. R. Zhao, et al., X. M. Yang\*, K. J. Yuan\*, *Sci. Adv.* 2021, 7, eabg7775.
- [5] Y. R. Zhao, Z. J. Luo, Y. Chang, et al., M. N. R. Ashfold\*, K. J. Yuan\*, X. M. Yang, *Nat. Commun.* 2021, 12, 4459. (Featured Article).
- [6] Chang, Y.; An, F.; Chen, Z. C.; et al.; Yuan, K. J.; Yang, X. M. *Nat. Commun.* 2021, 2021, 12, 6303 (Featured Article).

## 报告摘要

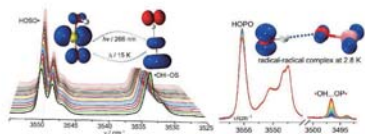
## 邀请报告

## 自由基复合物的低温光谱探测

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中间体作为连接反应物与产物的关键活性物种, 其直接光谱探测、结构与化学特性研究对于揭示反应的微观机制至关重要。我们采用低温基质隔离光谱探测装置, 联用高真空闪光热解与激光光解技术, 结合高精度理论计算对在有机合成、能源催化、大气污染、燃烧、星际化学等复杂过程中的重要瞬态活性中间体开展了光谱探测与相关反应机制的实验和理论研究。本报告将重点介绍通过“逆向合成”策略在超低温惰性基质中制备并表征典型自由基(OH, NH)与一氧化硫(OS)、一氧化磷(OP)和水分子发生放热复合反应过程中的关键中间体即“反应复合物”与“自由基对”, 在获取其指纹光谱数据的基础上, 结合同位素标记对动力学过程进行原位跟踪测量, 实现了低能垒( $< 1$  kcal/mol)与量子隧穿效应QMT动力学参数的准确测量[1-4]。该研究不仅表明低温基质隔离技术可用于分子间相互作用的研究, 而且也证实了“无势垒”的自由基放热复合存在中间体即存在分步反应机制。



图一: 低温基质中OH自由基复合物参与的动力学转化。

## References:

- [1] Li, X. L.; Zhu, B. F.; Wang, L. N. Trabelsi, T.; Francisco, J. S.; Zeng, X. Q. Manuscript in preparation.
- [2] Chu, X. X.; Qian, W. Y.; Lu, B.; Wang, L. N.; Qin, L.; Li, J.; Rauhut, G.; Trabelsi, T.; Francisco, J. S.; Zeng, X. Q. *Angew. Chem. Int. Ed.* 2020, 59, 21949–21953.
- [3] Chen, C. Y.; Lu, B.; Zhao, X. F.; Qian, W. Y.; Liu, J.; Trabelsi, T.; Francisco, J. S.; Qin, J.; Li, J.; Wang, L. N.; Zeng, X. Q. *J. Am. Chem. Soc.* 2020, 142, 2175–2179.
- [4] Wu, Z.; Chen, C. Y.; Liu, J.; Lu, Y.; Xu, J.; Liu, X. Y.; Cui, G. L.; Trabelsi, T.; Francisco, J. S.; Mardyukov, A.; Eckhardt, A. K.; Schreiner, P. R.; Zeng, X. Q. *J. Am. Chem. Soc.* 2019, 141, 3361–3365.

## 报告摘要

## 邀请报告

## Dynamics of triplet-pair states in singlet fission

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By converting a photo-excited singlet state into two triplet states, singlet fission holds the potential to break the efficiency limit in single-junction photovoltaic device. A doubly-excited triplet-pair state has been proposed as the key intermediate connecting singlet and two free triplets (i.e.,  $S_1 \rightarrow {}^1(TT) \rightarrow T_1 + T_1$ ) [1]. Nevertheless, the mechanism underlying the formation and dissociation of the  ${}^1(TT)$  state remains elusive. Using transient magneto-optical spectroscopy, we have identified a spatially separated triplet-pair state ( ${}^1(T...T)$ ) which enables the dissociation of  ${}^1(TT)$  states in both inter- and intra-molecular singlet fission systems [2-3]. Using two-dimensional electronic spectroscopy [4], we have observed that coherent vibronic coupling significantly promotes the formation of  $S_1 \rightarrow {}^1(TT)$  in heterodimer systems. Our findings uncover the mechanism underpinning TT formation and dissociation which may guide the search of singlet fission materials toward practical applications.

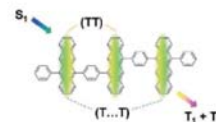


Figure 1: Adjacent and separated triplet-pair states involving in singlet fission.

**Acknowledgements:** This work has the support of National Natural Science Foundation.

## References

- [1] K. Miyata et al., *Chem. Rev.* 119, 4261 (2019).
- [2] Z. Wang et al., *Nat. Chem.* 13, 559 (2021).
- [3] R. Wang et al., *Nat. Commun.* 6, 8602 (2015).
- [4] W. Zhu et al., *Opt. Express* 25, 021115 (2017).



## 报告摘要

## 邀请报告

## 微液滴气液界面自发“奇特”的化学反应

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摘要正文: 水常常被认为是一种稳定且相对惰性的溶剂, 但近年来的许多研究却表明, 微米尺度的小水滴, 如云彩和雾滴等微液滴, 具有许多与体相溶液截然不同的独特性质。例如, 微液滴能够加速一些在体相溶液中进行得较慢的反应, 速度提升可达2到6个数量级; 又如, 微液滴还能触发一些原本无法在体相溶液中进行反应, 尤其是自发产生的自由基及其引发的氧化还原反应。许多现象表明, 微液滴中很可能存在有羟基自由基和自由电子, 赋予了微液滴氧化性还原性兼具、矛盾而又统一的奇特性质。该汇报记录了张新星课题组近年来在微液滴气液界面自发的自由基反应的新进展。[1-4]

## 参考文献

1. Chu Gong; Danyang Li; Xilai Li; Dongmei Zhang; Dong Xing; Lingling Zhao; Xu Yuan; Xinxing Zhang; Spontaneous Reduction-Induced Degradation of Viologen Compounds in Water Microdroplets and its Inhibition by Host-Guest Complexation, *J. Am. Chem. Soc.*, 2022, 144, 3510-3516.
2. Lingling Zhao; Xiaowei Song; Chu Gong; Dongmei Zhang; Ruijing Wang; Richard N. Zare; Xinxing Zhang; Sprayed Water Microdroplets Containing Dissolved Pyridine Spontaneously Generate the Unstable Pyridyl Radical Anion, *Proc. Natl. Acad. Sci. U.S.A.*, 2022, 119, e2200991119.
3. Dong Xing; Yifan Meng; Xu Yuan; Shuihui Jin; Xiaowei Song; Richard N. Zare; Xinxing Zhang; Capture of Hydroxyl Radicals by Hydronium Cations in Water Microdroplets, *Angew. Chem. Int. Ed.* 2022, e202207587
4. Dongmei Zhang, Xu Yuan, Chu Gong, Xinxing Zhang, High electric field on water microdroplets catalyzes spontaneous and ultrafast oxidative C-H/N-H cross-coupling. *J. Am. Chem. Soc.*, 2022, 10.1021/jacs.2c07385

## 报告摘要

## 邀请报告

## Study on chemical reaction kinetics of single droplets suspended by optical tweezers

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Optical tweezers technology can suspend a single droplet of 2-10 microns. Using stimulated Raman spectroscopy, it can accurately measure the radius change of the droplet, which provide the kinetic data of SO<sub>2</sub> gas reacted on/in ammonium sulfate single droplet under controlled reaction conditions. Thus we can draw out the influence of droplet concentration, pH, transition metal ion catalysis, relative humidity and other factors on the reaction rate, determine the surface and internal reaction rate of the droplet, and reveal the mechanism of rapid transformation of sulfate from haze pollution in China.

**Acknowledgements:** This work has the support of NSFC No. 42127806

## References

- [1] Z. Chen, P. Liu, W.G. Wang, etc., *Environ. Sci. Technol.* 56, 7637–7646 (2022).



## 报告摘要

## 邀请报告

## Transformation of methane mediated by atomic clusters

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Methane, the principal constituent of natural gas, represents an important C1 feedstock for production of value-added chemicals. However, the activation and transformation of methane under mild conditions have been referred to as one of the "holy grails" in contemporary chemistry owing to the inertness of CH<sub>4</sub> molecule. The design of catalysts for efficient methane conversion requires the fundamental knowledge about the mechanistic details of elementary reactions, structure-activity relationship of active sites, and the role of interface and ligands tuning the activity and selectivity. Atomic clusters composed of limited numbers of atoms can serve as ideal models for the active centers of "real-life" catalysts. In recent years, we prepared a series of metal-based clusters and measured their reactivity toward CH<sub>4</sub> by using mass spectrometric experiments. The structural characterization of cluster species has also been conducted. In this conference, the structural characteristics of active clusters that can mediate activation and transformation of methane at low temperatures will be presented. The catalytic reactions for co-conversion of CH<sub>4</sub> with other inert molecules mediated by clusters with the assistance of high temperatures, collision-induced dissociation, and photo-irradiation will also be emphasized. <sup>34</sup>

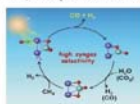


Figure 1: Photoassisted steam reforming and dry reforming of methane to syngas catalyzed by Rh<sub>n</sub>VO<sub>m</sub> clusters at room temperature.

**Acknowledgements:** This work has the support of the National Natural Science Foundation of China (92061115) and the Youth Innovation Promotion Association of the Chinese Academy of Sciences (2018041).

## References

- [1] X.-L. Ding, X.-N. Wu, Y.-X. Zhao, S.-G. He, *Acc. Chem. Res.*, 45: 382 (2012).
- [2] Y.-X. Zhao, M.-M. Wang, X.-L. Ding, S.-G. He, *Angew. Chem. Int. Ed.*, 58: 8002 (2019).
- [3] Y.-X. Zhao, Z.-Y. Li, Y. Yang, S.-G. He, *Acc. Chem. Res.*, 51: 2603 (2018).
- [4] Q. Chen, Y.-X. Zhao, L.-X. Jiang, J.-J. Chen, S.-G. He, *Angew. Chem. Int. Ed.*, 57: 14134 (2018).
- [5] Y. Yang, B. Yang, Y.-X. Zhao, L.-X. Jiang, Z.-Y. Li, Y. Ren, H.-G. Xu, W.-J. Zheng, S.-G. He, *Angew. Chem. Int. Ed.*, 58: 17287 (2019).
- [6] Y.-X. Zhao, B. Yang, H.-F. Li, Y. Zhang, Y. Yang, Q.-Y. Liu, H.-G. Xu, W.-J. Zheng, S.-G. He, *Angew. Chem. Int. Ed.*, 59: 21216 (2020).
- [7] Y. Yang, Y.-K. Li, Y.-X. Zhao, G.-P. Wei, Y. Ren, K. R. Asmis, S.-G. He, *Angew. Chem. Int. Ed.*, 60: 13788 (2021).
- [8] Y.-X. Zhao, X.-G. Zhao, Y. Yang, M. Ruan, S.-G. He, *J. Chem. Phys.*, 154: 180901 (2021).

## 报告摘要

## 邀请报告

## Vibrationally-resolved spectra and electron dynamics in organic aggregates simulated from a non-Markovian stochastic Schrödinger equation

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A non-Markovian stochastic Schrödinger equation [1,2] is presented for the calculation of absorption spectra of molecular aggregates immersed in harmonic quantized vibrational modes. The feasibility and the validity of newly proposed method are affirmed in the analytical monomer spectra. In the simulations, various types of local excitations, charge-transfer (CT) excitations, and exciton-phonon couplings are explicitly included in a comprehensive model Hamiltonian, parameterized by first-principles calculations, together with a diabatic strategy of the fragment particle-hole densities [3]. The applications to Zinc Phthalocyanine aggregates [4,5] clarify that the two absorption bands in the Q-band region observed in experiments can be assigned to the contribution from the CT-mediated interactions, rather than the mixtures of different-type aggregates, as prevalently assumed. From the investigation of the decoherence process after optical excitation, it is found that CT states can induce coherence regeneration as the time scale of charge separation is much faster than that of the vibration-induced decoherence. However, they would instead boost the decoherence process as the two time scales become comparable.

**Acknowledgements:** This work has the support of National Science Foundation of China (22033006, 21833006) and China Postdoctoral Science Foundation (294469).

## References

- [1] Y. Ke and Y. Zhao, *J. Chem. Phys.*, 146, 174105 (2017).
- [2] S. Feng, Y. Wang, Y. Ke, W. Z. Liang, and Y. Zhao, *J. Chem. Phys.*, 153, 034116 (2020).
- [3] Y. Wang, S. Feng, W. Z. Liang, and Y. Zhao, *J. Phys. Chem. Lett.*, 12, 1032 (2021).
- [4] S. Feng, Y. Wang, W. Z. Liang, and Y. Zhao, *J. Phys. Chem. A*, 125, 2932 (2021).
- [5] S. Feng, Y. Wang, W. Z. Liang and Y. Zhao, *Phys. Chem. Chem. Phys.*, 24, 2974 (2022).

## 报告摘要

## 邀请报告

## Excited state processes in organic microlaser materials

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The abundant excited state processes of organic materials provide a possible means of constructing four-level excited state systems required for population inversion; and the various spectral characteristics of the material in the stimulated state are beneficial for in-depth study of the excited state dynamics of different organic molecules. Organic molecules absorb photons and generate excited states localized on a single molecule—Frenkel excitons, whose binding energy is an order of magnitude higher than Wannier excitons of inorganic materials. Frenkel excitons have high room temperature stability, strong spatial confinement, and can strongly couple with photons to form a new quantum state—exciton polarized exciton. The formation of exciton polariton can significantly reduce the laser threshold. Therefore, a zero-threshold laser can be achieved through reasonable material design.

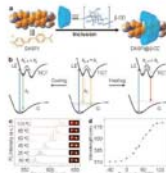


Figure 1: Broadband tunable organic microlasers based on intramolecular charge transfer

**Acknowledgements:** This work has the support of Ministry of Science and Technology of China and National Natural Science Foundation of China.

**References**

- [1] J. Tang, J. Zhang, Y. Lv, H. Wang, F. F. Xu, C. Zhang, L. Sun, J. Yao, Y. S. Zhao. Nat. Commun. 12, 3265 (2021).
- [2] C. Zhang, H. Dong, C. Zhang, Y. Fan, J. Yao, Y. S. Zhao. Sci. Adv. 7, eabh3530 (2021).
- [3] J. Zhao, Y. Yan, Z. Gao, Y. Du, H. Dong, J. Yao, Y. S. Zhao. Nat. Commun. 10, 870 (2019).
- [4] W. Zhang, J. Yao, Y. S. Zhao. Acc. Chem. Res. 49, 1691-1700 (2016).
- [5] C. H. Zhang, C. L. Zou, H. Dong, Y. Yan, J. Yao, Y. S. Zhao, Sci. Adv. 3, e1700225 (2017).
- [2] F. L. Author, H.-G. Test, book title (publishing company, place, year).

## 报告摘要

## 邀请报告

## 光电转换半导体激发态电子-晶格耦合极化动力学

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具有低维晶格结构的新型半导体材料是当前光电转换的研究热点。其中, 半导体材料吸收光后的激发态动力学和性质直接决定了光电转换器件的性能优化和设计原理, 具有重要的指导作用。在传统的三位共价半导体中, 如Si和GaAs中, 由于较弱的电子-晶格相互作用, 自由电子图像常常足够描述激发态载流子的动力学行为, 晶格的性质可以忽略。但是, 在这些新型的低维晶格半导体中, 由于软的晶格或晶格间弱相互作用的存在, 常常会出现来强的非谐性晶格振动和电-声子相互作用, 电子的运动将和晶格强烈耦合在一起, 形成极化子, 类似于固体中的溶剂化效应, 传统的自由电子图像不再成立。耦合的电子-晶格运动将从本质上改变激发态载流子动力学行为, 产生新的物理化学性质。在这个报告中, 我们将以二维铅卤八面体和层状碘化铪材料为例, 通过显微超快光谱手段, 分别揭示激发态耦合的电子-晶格运动, 大(小)极化子的形成, 以及对激发态载流子性质的影响, 包括能量损失、反常的激子自旋动力学、抑制的多激子俄歇作用等。

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**References**

- [1] Tao, W.; Zhou, Q.; Zhu, H., Dynamic polaronic screening for anomalous exciton spin relaxation in two-dimensional lead halide perovskites. Sci. Adv. 2020, 6 (47), eabb7132.
- [2] Tao, W.; Zhang, C.; Zhou, Q.; Zhao, Y.; Zhu, H., Momentarily trapped exciton polaron in two-dimensional lead halide perovskites. Nat. Commun. 2021, 12 (1), 1400.

## 报告摘要

## 口头报告

## 表观遗传核酸的激发态动力学研究

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核酸是地球上绝大多数生命体的遗传信息载体。研究表明, 核酸分子中存在着多种动态表观遗传修饰, 这些修饰不仅改变核酸的分子结构, 还在基因表达、生长发育、生理功能调控、癌症发病等生理过程中起着重要的作用。在这其中, 甲基化修饰是最主要的核酸表观遗传修饰。<sup>1</sup>已有报道表明, 核酸甲基化修饰的程度会显著影响其光化学损伤及修复, 但是该过程的微观化学反应机理还未明确。我们采用时间分辨光谱技术, 自下而上的对一系列表观遗传的核酸碱基、二聚体、DNA链的激发态动力学进行了系统的研究。基于我们的实验结果, 我们发现总结了表观遗传修饰对核酸碱基激发态特性的影响规律。并在此基础上, 揭示了表观遗传修饰碱基对DNA中的电子转移、能量转移以及进一步地DNA的光损伤机制的影响。该工作为后续开展核酸动态化学修饰精确调控以及开发相关光动力学疗法药物奠定了理论基础。

## 参考文献

1. Smith, Z. D.; Meissner, A., DNA methylation: roles in mammalian development. *Nature Reviews Genetics* 2013, 14 (3), 204-220.
2. Zhou, Z.; Zhou, X.; Wang, X.; Jiang, B.; Li, Y.; Chen, J.; Xu, J., Ultrafast Excited-State Dynamics of Cytosine Aza-Derivative and Analogues. *J. Phys. Chem. A* 2017, 121 (14), 2780-2789.
3. Wang, X.; Zhou, Z.; Tang, Y.; Chen, J.; Zhong, D.; Xu, J., Excited State Decay Pathways of 2'-deoxy-5-Methylcytidine and Deoxycytidine Revisited in Solution: A Comprehensive Kinetic Study by Femtosecond Transient Absorption. *J. Phys. Chem. B* 2018, 122, 7027-7037.
4. Wang, X.; Yu, Y.; Zhou, Z.; Liu, Y.; Yang, Y.; Xu, J.; Chen, J., Ultrafast Intersystem Crossing in Epigenetic DNA Nucleoside 2'-Deoxy-5-formylcytidine. *J. Phys. Chem. B* 2019, 123 (27), 5782-5790.
5. Zhou, Z.; Hu, Z.; Zhang, X.; Jia, M.; Wang, X.; Su, H.; Sun, H.; Chen, J.; Xu, J., pH Controlled Intersystem Crossing and Singlet Oxygen Generation of 8-Azaadenine in Aqueous Solution. *ChemPhysChem* 2019, 20 (5), 757-765.
6. Zhou, Z.; Wang, X.; Chen, J.; Xu, J., Direct Observation of Intramolecular Charge Transfer State in Epigenetic Nucleobase N6-methyladenine. *Phys. Chem. Chem. Phys.* 2019.
7. Fu, L.; Wang, Z.; Liu, Y.; Wang, X.; Xu, R.; Liu, W.; Chen, J.; Xu, J., Observation of triplet  $nn^*$  state in ultrafast intersystem crossing of 6-azathymine. *J. Photochem. Photobiol. A: Chem.* 2020, 396, 112491.
8. Xu, R.; Hu, Z.; Wang, X.; Liu, Y.; Zhou, Z.; Xu, J.; Sun, Z.; Sun, H.; Chen, J., Intramolecular Charge Transfer in 5-Halogen Cytidines Revealed by Femtosecond Time-Resolved Spectroscopy. *J. Phys. Chem. B* 2020, 124 (13), 2560-2567.

## 报告摘要

## 口头报告

## The effect of spin-orbit interaction in the F+HD→HF+D reaction

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Since electron spin was discovered, it is found that the couplings between the electron spin and orbital angular momentum could lead to many interesting phenomena. In chemical reactions, these couplings can result in the splitting of partial waves which may make some fine structures of partial waves arise.

Using a high-resolution imaging technique, the rotational-state-resolved differential cross sections of the products D atoms from F (<sup>2</sup>P<sub>1/2</sub>) + HD (v=0, j=0) reaction were detected. A peculiar horseshoe-shaped structure was observed in the forward scattering direction. Compared with quantum dynamics calculation results with or without spin-orbit interaction, it showed that only the theoretical results from the model that includes the full spin-orbit effect can agree with the experimental results. Further analysis indicated that the couplings between electron spin and orbital angular momentum split the partial waves and substantially altered the interference pattern of the F+HD reaction which led to the peculiar horseshoe-shaped structure. This finding provided a distinctive example of how spin-orbit interaction can effectively influence reaction dynamics.

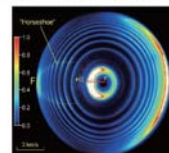


Figure 1: Experimental image of the D-atom product from the F + HD → HF + D reaction at a collision energy of 2.10 kcal/mol.

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## References

- [1] Wentao Chen, Ransheng Wang, etc., *Science*, 371 936 (2021).

## 报告摘要 口头报告

## Free-electron laser based Infrared absorption spectroscopy and dissociation dynamics study

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Infrared (IR) spectroscopy could provide figure print information of species and be used to characterize new species or identify and verify known and unknown samples. IR-VUV two-color ionization method, monitoring the variation of ion signal with and without IR laser irradiating, could identify the IR absorption of samples. The photon energy of VUV was typically selected to be near the threshold ionization energy of the sample to ensure a better signal-to-noise ratio. Therefore, the VUV light source should be tunable when applied to different samples, and the peak intensity of the VUV laser should be strong enough when this method is applied to low concentration species such as free radicals. Free electron laser (FEL) perfectly meets such needs.

Combining the VUV laser from Dalian Coherent Light Source with a tunable OPO/OPA IR laser, we measured the IR absorption of dihydroxyacetone in the range from 2700 to 4700  $\text{cm}^{-1}$ . Comparing the IR absorption obtained from monitoring the  $\text{C}_3\text{H}_5\text{O}_2^+$  with that obtained from monitoring the dissociation product  $\text{C}_2\text{H}_3\text{O}^+$ , we find some vibrational mode excitation of dihydroxyacetone does not promote the dissociation of  $\text{C}_3\text{H}_5\text{O}_2^+$ , even though the total energy is sufficient for this process. We also measured the IR absorption of  $\text{CH}_2\text{CHOO}$  Criegee intermediate (CIs) in the IR photon energy range of 2700-3200  $\text{cm}^{-1}$ , with some absorption peaks primitively attributed to the absorption of syn- $\text{CH}_2\text{CHOO}$  and others to that of anti- $\text{CH}_2\text{CHOO}$ .

**Acknowledgements:** This work has the support of the National Natural Science Foundation of China (21873098, 22288201); the Chinese Academy of Sciences (GJJSTD20220001, XDB17000000); the International Partnership Program of the Chinese Academy of Sciences (121421KYSB20170012) and the Liaoning Revitalization Talents Program (XLYC1807248).

## 报告摘要 口头报告

## Non-adiabatic molecular reaction dynamics in diabatic representation

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The study of non-adiabatic chemical processes has long been a frontier in molecular reaction dynamics. In order to accurately study the non-adiabatic processes, it is far more advantageous to work within a diabatic representation than an adiabatic representation. We have developed a fitting-and-diabatizing method based on artificial neural networks, which is one of the most accurate methods of diabaticization [1]. Based on accurate diabatic representation, molecular properties [2] and spin-orbit couplings [3] can also be diabaticized. These developments ultimately provide a complete diabatic representation, that is all the electronic structure data needed for the study of non-adiabatic processes can be analytically expressed within a unified diabatic representation. Diabatic representation also provides a complete description of quantum effects in non-adiabatic chemical processes. For example, by taking advantage of the diabatic representation of H<sub>2</sub>, we have observed and confirmed the geometric phase effect in the H+HD reaction [4].

Non-adiabatic processes are ubiquitous in chemistry, which are facilitated by either conical intersections (internal conversion) or spin-orbit couplings (intersystem crossing). In addition, light-matter interactions also lead to non-adiabatic events (light-induced conical intersections). All these non-adiabatic processes can be studied within the complete diabatic framework. Therefore, we can extend the study of non-adiabatic chemical processes in molecular reaction dynamics to a broader range of topics, which include the competition between internal conversion and intersystem crossing, and the light-induced conical intersections.

## References

- [1] Y. Guan, H. Guo, and D. R. Yarkony, *J. Chem. Phys.*, 150 214101 (2019).
- [2] Y. Guan, H. Guo, and D. R. Yarkony, *J. Chem. Theory Comput.*, 16 302 (2020).
- [3] Y. Guan and D. R. Yarkony, *J. Phys. Chem. Lett.*, 11 1848 (2020).
- [4] D. Yuan, Y. Guan, W. Chen, H. Zhao, S. Yu, C. Luo, Y. Tan, T. Xie, X. Wang, Z. Sun, D. H. Zhang, and X. Yang, *Science*, 362 1289 (2018).



## 报告摘要 口头报告

Mechanistic Studies of Hydrogen Production on TiO<sub>2</sub>Rulin Sun<sup>1</sup>, Xinlu Liu<sup>2</sup>, Hongjun Fan<sup>2</sup>, Qing Guo<sup>1\*</sup><sup>1</sup>Department of Chemistry, Southern University of Science and Technology, Shenzhen, Guangdong, 518055, P. R. China<sup>2</sup>State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, CAS, Dalian, Liaoning, 116023, P. R. China

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TiO<sub>2</sub> has attracted enormous attentions, because of its potential applications, especially in the hydrogen production from water splitting, which provides a feasible way for human to obtain clean energy. In order to better understand the mechanism of hydrogen production, more and more works around the TiO<sub>2</sub> single crystal surface, especially the model TiO<sub>2</sub>(110) surface. Therefore, the investigation of fundamental processes of hydrogen production on TiO<sub>2</sub> surfaces plays an important role in the development of new catalysts to achieve hydrogen energy source from water splitting. Combination programmed desorption spectroscopy (TPD), scanning tunneling microscopy (STM) and density functional theory (DFT) calculation, the fundamental processes of hydrogen production on rutile TiO<sub>2</sub>(110) with formate, Au cluster, Pt cluster modification have been studied systematically.<sup>1-5</sup> These work provides a new insight in H<sub>2</sub> production from H<sub>2</sub>O and renewables with TiO<sub>2</sub> catalysts, which may be applicable to H<sub>2</sub> production on metal-oxide catalysts.

**Acknowledgements:** These work has the support of the National Key R&D Program of China (Grant No. 2018YFE0203002), the National Natural Science Foundation of China (Grant No. 22103031, 22173041 and 21873096), the Strategic Priority Research Program of Chinese Academy of Sciences.

## References

- [1] R. Sun, R. Wang, etc., Hydrogen Production on Pt/TiO<sub>2</sub>: Synergistic Catalysis between Pt Clusters and Interfacial Adsorbates. *J. Phys. Chem. Lett.* 13, 3182-3187 (2022).
- [2] F. Li, X. Chen, etc., Xueming Yang. Hydrogen Production via Methanol Photocatalysis on Au/Rutile-TiO<sub>2</sub>(110). *J. Phys. Chem. C* 124, 26965-26972 (2020).
- [3] Z. Geng, X. Jin, etc., Low-Temperature Hydrogen Production via Water Conversion on Pt/TiO<sub>2</sub>. *J. Phys. Chem. C* 122, 10956-10962 (2018).
- [4] C. Xu, R. Wang, etc., Enhanced Hydrogen Production from Methanol Photolysis on a Formate-Modified Rutile-TiO<sub>2</sub>(110) Surface. *J. Phys. Chem. C*, 122, 10956-10962 (2018).
- [5] C. Xu, W. Yang, etc., Molecular Hydrogen Formation from Photocatalysis of Methanol on TiO<sub>2</sub>(110). *J. Am. Chem. Soc.*, 135, 10206-10209 (2013).

## 报告摘要 口头报告

## Hydrogen Generation Catalyzed by Isolated and Supported Metal Clusters

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Looking for sustainable and environment-friendly alternatives to fossil fuels has become a grand challenge worldwide, which has stimulated extensive efforts to develop efficient energy conversion technologies. Hydrogen is a convenient, safe, and versatile fuel source, and can be converted to a desired form of energy without the emission of greenhouse gases and pollutants.

Methanol is a green and convenient energy source for methanol fuel cells, i.e., the methanol economy, in which one important step is methanol dehydrogenation to produce hydrogen. To explore low cost, selective, and efficient catalyst for methanol dehydrogenation, a prerequisite is to understand the reaction pathways and the underlying catalytic mechanisms at the atomistic level, for which capturing and characterizing the fleeting reaction intermediates and active sites are crucial. Here, I will present our effort in past years towards this goal by studying the reactions of metal clusters with methanol in a low-pressure collision cell and mass spectrometry, as well as the reactions of supported vanadium atoms/clusters towards methanol and/or water.

**Acknowledgements:** This work has the support from National Natural Science Foundation of China, the KU Leuven Research Council, and Xi'an Jiaotong University.

## References

- [1] Hou\*, et al. *Angew. Chem. Int. Ed.* 60, 4756-4763 (2021).
- [2] Hou\*, et al. *Angew. Chem. Int. Ed.* 60, 27095-27101 (2021).
- [3] Li, ..., Hou\*. *Cell Rep. Phys. Sci.* 3, 100910 (2022).

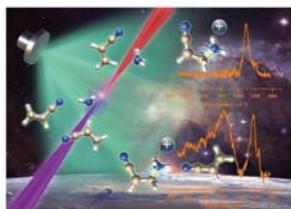
## 报告摘要

## 口头报告

## 星际分子团簇中的化学动力学

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生物光子学研究院, 华南师范大学, 510631  
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团簇是由几个、几十个乃至上千个原子、分子或离子通过物理或化学结合力组成的相对稳定的微观或亚微观聚集体。气相中的分子团簇是研究生物分子识别、环境污染物的形成以及星际分子的演化过程的模型体系。本报告首先简单综述了人们基于飞行时间质谱仪器, 研究超声分子束中分子团簇的结构和光电离动力学过程的研究进展<sup>[1-3]</sup>之后重点报告了本课题组在近年来开展与星际相关的分子及其分子团簇<sup>[4-6]</sup>。在真空紫外单光子电离诱导下所发生的光电离反应动力学过程和光谱探测, 研究了星际分子丙烯腈与其他星际小分子如氨分子、甲醇分子以及水分子等形成的分子团簇和离子团簇, 发现在118nm单光子电离诱导后形成的团簇离子中, 丙烯腈和小分子单体之间可能形成了新的C-N化学键<sup>[4]</sup>由此形成新的离子化合物。应用IR/VUV光谱方法并结合理论计算获得了形成新C-N化学键相关的光谱学证据。这一研究结果对于我们了解早期星际分子的演化过程以及星际中生物大分子的形成都有着重要的参考价值和科学意义。



## 参考文献

1. J. Stevenson, J. Lunine and P. Clancy, *Sci. Adv.*, 2015, 1(1), e1400067.
2. N. Balucani, *Chem. Soc. Rev.*, 2012, 41, 5473-5483.
3. Y. Hu, J. Guan and E. R. Bernstein, *Mass Spectrom. Rev.*, 2013, 32, 484-501.
4. Y. Li, W. Song, N. Jiang, Z. Zhang, M. Xie, Y. Hu, *Spectrochim. Acta, Part A*, 2020, 226, 117620.
5. F. Sun, M. Xie, Y. Zhang, W. Song, X. Sun, Y. Hu, *Phys. Chem. Chem. Phys.*, 2021, 23, 9672-9678.

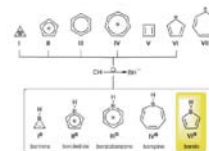
## 报告摘要

## 口头报告

## Synthesize and characterize of novel boron heterocyclic radicals in inert matrices

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Boron-containing heterocyclic radicals play an important role in chemical synthesis and medical chemistry, owing to their unique geometric/electronic structures and chemical reactivities. Although many related methods have been developed, the synthesis of boron heterocyclic compounds and the corresponding radicals remains challenging, because these compounds are usually very reactive. Previous research has suggested that boron atom selectively inserted into the C=C double bond, rather than the lower activation energy required C-H bond in forming organoboron radicals, during the reaction of boron atoms with ethylene molecule under matrix isolated condition. This anomalous discovery opens the door to the synthesize method of boron-containing heterocyclic radicals. In the present study, novel boron heterocyclic radicals were isolated under low-temperature matrix isolation conditions and identified by infrared spectra in the reaction of boron atom with benzene, cyclopentene, cyclohexene, and cycloheptene. These results clearly show that the boron atom can insert into the carbon-carbon double bonds and form new borole derivatives through the photo-induced multiple hydrogen-atom transfer and rearrangement reactions. The present findings give new insight into the future design and synthesis of the corresponding boron heterocyclic compounds.



## References

- [1] Y. Su and R. Kinjo, *Chem. Soc. Rev.*, 2019, 48, 3613-3659.
- [2] J. Jian, H. Lin, M. Luo, M. Chen, and M. F. Zhou, *Angew. Chem. Int. Ed.* 2016, 55, 8371-8374

## 报告摘要

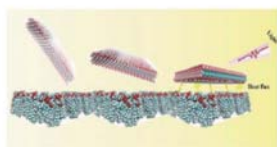
## 口头报告

## 光热或光化学治疗: MXene 界面电子超快动力学研究

Jiebo Li (李介博)<sup>1\*</sup><sup>1</sup>北京航空航天大学, 医工交叉创新研究院, 北京市海淀区学院路 37 号, 100191.

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MXene作为新型二维材料, 由于其在近红外区优异的光吸收能力, 在光治疗领域具有广阔的应用前景。报告从MXene在生物医学工程应用中遇到的问题出发, 提炼光治疗的物理化学问题—MXene吸收红外光后的动力学行为以及调控机制。报告围绕MXene电子激发态超快动力学的分析研究, 系统介绍MXene界面上的红外光驱动热电子的能量转化和电子转移过程, 阐述其光-电子-声子多个过程调控因素, 并结合分子动力学从核心物理化学角度理解MXene作为新型光治疗材料的作用机制, 并依据超快动力学研究开展了激光光谱杀菌、疫苗递送、超快红外激光器等诸多新型应用。



**Acknowledgements:** This work has the support of NSFC(21803006, 22073003).

## References

- [1] Li, J.; Zhang, Q.; Yan, L.; et al. *Adv. Mater. Interfaces* 2019, 6 (23): 1901461.
- [2] Wu, D.; Zhao, R.; Chen, Y.; et al. *Phys. Chem. Chem. Phys.* 2021, 23:3341.
- [3] Wu, F.; Chen, H.; Wang, W. et al. *Sci. China. Mater.* 2021, 64(3): 748.
- [4] Li, J.; Qin, R.; Yan, L.; et al. *Inorg. Chem.* 2019, 58(11): 7285.
- [5] Li, J.; Chi, Z.; Qin, R.; et al. *J Phys. Chem. C* 2020, 124(19): 10306.
- [6] Zhang, Q.; Chen, Y.; Zhang, Y. et al. *J. Phys. Chem. Lett.* 2020, 11: 9521.
- [7] Zhang, Q.; Yan, L.; Yang, M. et al. *J Phys. Chem. C* 2020, 124(11): 6441.
- [8] Zhao, R. et al. *Phys. Chem. Chem. Phys.* 2021, 23:16998.
- [9] Shang, Ce, et al. *J. Alloys Comp.* 2022, 918:165580.

## 报告摘要

## 口头报告

## Broadband chirped-pulse Fourier transform microwave spectroscopy probing the structures and nuclear tunneling of molecular clusters

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Spectroscopic studies of molecular clusters in gas-phase can benchmark theoretical methods for modeling intermolecular interactions. The key features of molecular clusters, such as their conformational flexibility and subtle noncovalent interactions, pose major challenges to spectroscopic techniques. Internal motions encoding their nature into the spectral splitting often prevent the experimental accuracy or, if recognizable, assignment. Rotational spectroscopy holds the possibility of true structure determination where analysis of the spectra of isotopic species provides actual atom positions in the 3D structure. Since its invention in 2008, the broadband chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy has transformed the field of high-resolution molecular spectroscopy[1]. The technique with collection over 10 GHz bandwidth spectrum in a single shot (several microseconds) enables faster-than-ever structure determination of increasing complex species (but spectral assignment is still a tough job). Herein, our new-build 2-8GHz CP-FTMW spectrometer at Fudan university, and some examples to probe the molecular structures, interactions and quantum tunneling will be discussed[2].

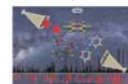


Figure 1: Scheme of molecular complexes probed by CP-FTMW spectroscopy.

## References

- [1] G. G. Brown, B. H. Pate, et al., *Rev. Sci. Instrum.* 79, 053103 (2008).
- [2] W. Li, et al., *Angew. Chem. Int. Ed.* 60, 25674-25679 (2021). *Angew. Chem. Int. Ed.* 60, 5323-5330 (2021). *Angew. Chem. Int. Ed.* 58, 859-865 (2019). *Angew. Chem. Int. Ed.* 58, 8437-8442 (2019). *Angew. Chem. Int. Ed.* 57, 13853-13857 (2018).

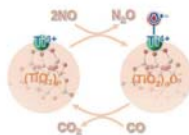
## 报告摘要

## 口头报告

## 金属团簇催化转化CO和NO反应机制研究

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CO与NO ( $2\text{CO} + \text{NO} \rightarrow 2\text{CO}_2 + \text{N}_2$ )共转化可将两种有毒气体转化为无毒的 $\text{CO}_2$ 和 $\text{N}_2$ ,是汽车尾气净化、工业废气处理等过程的重要反应。对相关催化活性中心的结构和催化反应机制的深入认识是实现低温高效、精准设计催化剂的科学基础。原子团簇可作为模拟异相催化剂上活性位的理想模型,用于研究相关催化转化反应的机制。但N-O键较强(6.55 eV),在气相团簇领域,相关研究以NO在团簇上的分子或解离吸附反应为主,人们对异核金属团簇上不同金属之间协同催化作用促进N-O解离和N-N耦合等关键基元步的认识还很有限。近期,我们利用团队最新研制的双离子阱反应器耦合反射式飞行时间质谱实验研究了系列同核及异核金属团簇催化转化CO和NO的反应,并借助量子化学理论模拟揭示了催化反应机制,取得了系列研究进展[1,2]。发现了系列中性铈氧化物团簇上暴露的Rh-Al极性键对于NO活化、解离以及N-N耦合的关键催化作用[1];发现系列钛氧化物团簇阴离子 $(\text{TiO}_2)_n^-$ 上单电子局域的 $\text{Ti}^{IV}$ 离子催化转化NO生成 $\text{N}_2\text{O}$ 的单电子还原机理( $2\text{NO} + e^- \rightarrow \text{N}_2\text{O} + \text{O}^-$ ) (图1)[2]。

图1: 钛氧化物团簇 $(\text{TiO}_2)_n^-$ 催化转化CO和NO反应示意图。

**致谢:** 相关研究获得基金委优秀青年科学基金(22022308)和重大研究计划培育项目(21773254)、科技部重点研发项目(2021YFA1500704)以及中科院青促会优秀会员等项目资助(Y202007)。

## References

- [1] J. J. Chen, X. N. Li, L. H. Mou, Q. Y. Liu, S. G. He, J. Mater. Chem. A, 10 6031 (2022).
- [2] J. J. Chen, Y. Z. Liu, Q. Y. Liu, X. N. Li, S. G. He, ACS Catal., 12 8768 (2022).
8. Xu, R.; Hu, Z.; Wang, X.; Liu, Y.; Zhou, Z.; Xu, J.; Sun, Z.; Sun, H.; Chen, J., Intramolecular Charge Transfer in 5-Halogen Cytidines Revealed by Femtosecond Time-Resolved Spectroscopy. J. Phys. Chem. B 2020, 124 (13), 2560-2567.

## 报告摘要

## 口头报告

## Hydration spectra and hydration number of organic and non-organic compounds in water by novel vibrational spectroscopy analysis method

Cheng Peng<sup>1</sup>, Chi Chen<sup>1</sup>, Zhi-Qiang Wang<sup>1</sup>, Lin Ma<sup>1</sup>, Rui-Ting Zhang<sup>1</sup>  
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The microstructure of aqueous solutions is very important, which is widely studied by various vibrational spectroscopy. However, the hydration spectra are overlapped though the spectra of water, thus the hydration structure and hydration number are difficult to be obtained through vibrational spectroscopy. Recent years, we proposed some novel spectroscopy analysis methods, such as the ratio vibrational spectroscopy, modified excess vibrational spectroscopy. Using these methods, the hydration spectra in the OH stretching region and OH bending stretching region were obtained in the aqueous solutions. The hydration number of various organic compounds and non-organic compounds in water is measured through these hydration spectra. The micro-structure of the aqueous solutions in various concentrations are also discussed through the hydration spectra and the hydration number. Some interesting structures were observed, for example, the cooperative interactions among the hydrophilic groups and hydrophobic groups.

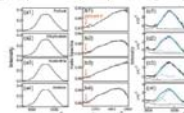


Figure 1: FTIR spectra (a), ratio spectra (b) and hydration spectra (c) of furfural (1), ethyl acetate (2), acetonitrile (3) and acetone in water.

**Acknowledgements:** This work has the support of NSFC((21473171,21703164) and NSF in Shanxi (2019JM-087, 2019JQ-047)

## References

- [1] Yu-xi Wang, Wei-duo Zhu, Ke Lin, et al, Journal of Raman Spectroscopy, 47 (2016)
- [2] Dor Ben-Amotz, Journal of the American Chemical Society, 141 (2019)



## 报告摘要 口头报告

Isotope effects and heavy-light-heavy reactivity oscillation in the Cl + CHD<sub>3</sub> reactionsShu Liu<sup>1</sup>, Xiaoxiao Lu<sup>1</sup>, Zhaojun Zhang<sup>1</sup>, and Dong H. Zhang<sup>1\*</sup><sup>1</sup>State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, Liaoning 116023, China.

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Previous experiments and theories have shown the existence of heavy-light-heavy (HLH) reactivity oscillation in the Cl + CH<sub>4</sub> reaction [1], and anticipated that similar oscillations should exist in many HLH reactions involving polyatomic reagents. However, the total reaction probabilities for Cl + CHD<sub>3</sub> → HCl + CD<sub>3</sub> exhibit only a step like feature, and the total reaction probabilities for Cl + CHT<sub>3</sub> → HCl + CT<sub>3</sub> do not show any structure at all. Here we report seven-dimensional state-to-state quantum dynamics studies for these two reactions on the FI-NN PES, and discuss the HLH reactivity oscillations and isotope effects in these two reactions.

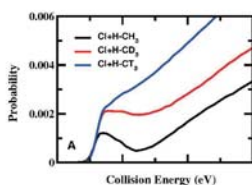


Figure 1:  $J=0$  total reaction probabilities for the initial ground rovibrational state as a function of collision energy of the three reactions.

**Acknowledgements:** This work has the support of NSFC.

## References

- [1] Z. Chen, J. Chen, R. Chen, T. Xie, X. Wang, S. Liu, G. Wu, D. Dai, X. Yang, D. H. Zhang, Reactivity oscillation in the heavy-light-heavy Cl + CH<sub>4</sub> reaction. PNAS 117, 9202-9207 (2020).

## 报告摘要 口头报告

## Zero-threshold Auger-enabled Electron Transfer Dynamics between Adjacent Quantum Wells in Two-Dimensional Layered Perovskites

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Two-dimensional (2D) Ruddlesden-Popper (RP) layered perovskites can naturally form multiple quantum wells (QWs), rendering promising applications in quantum and optoelectronic devices. Due to the strong quantum confinement effect, photogenerated exciton is confined in the perovskite QW plane. Although excellent inner layer carrier transport property has been reported,<sup>[1]</sup> interlayer (QW-to-QW) carrier transport is still difficult because of the energy barriers between organic ligands and perovskite layers, especially for type-I quantum well structures. Recently, Jin et al. have demonstrated Auger-assisted electron transfer between adjacent QWs in RP perovskites, which required high excitation power densities which is impractical in real applications.<sup>[2]</sup> Herein, we successfully designed a new series of type-I RP layered perovskites using organic ligands of cyclo-carbo-alkaneamine (C=3, 4, 5, 6). Ultrafast dynamics measurements revealed that both the 2D perovskites with cyclopropyl (C=3) and cyclobutyl (C=4) ligands display a blueshift of exciton bleach at longer time delays, which is attributed to the Stark Effect caused by the separation of photogenerated electrons and holes. Remarkably, the threshold excitation power density of such charge separation is much lower than that reported in the literatures, which is more suitable for photovoltaic devices that require efficient electron-hole separation.

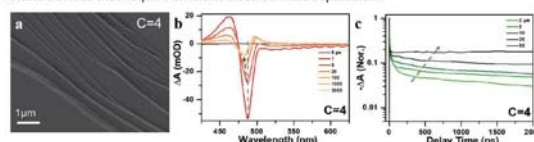


Figure 1 (a) SEM image, (b) ultrafast transient absorption spectra, and (c) ground state bleaching kinetics of C=4 perovskites under different excitation intensities at 400 nm.

**Acknowledgements:** This work is supported by the National Science Foundation of China (Grant No. 22073001) and the University Synergy Innovation Program of Anhui Province (GXXT-2021-049).

## References

- [1] Zhao C, Tian W, etc., J Am Chem Soc, 142, 15091-15097, (2020).  
[2] Yin Z, Leng J, W etc., J Am Chem Soc 143, 4725-4731, (2021).

## 报告摘要

## 口头报告

## Reaction dynamics of metal clusters

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With the development of experiment technology, researchers working in cluster science have been able to devise reliable methods to fabricate metal nanoparticles which are so small that their energy levels present a discrete spectrum allowing the stability and reactivity to be determined by the nature of geometric/electronic shells and the degree to which they are filled. Studies of reaction dynamics of metal clusters are thus important for understanding the properties of macroblock metals at reduced size as well as the active sites or stable structural units on metal surfaces [1-3].

We would like to contribute to this conference by sharing our recent advances in the metal cluster reactivities [4-9], including superatomic species of transition metal clusters of which interesting superatomic orbitals contributed by the d-bands. These studies are devoted to understanding the key scientific problems related to corrosion and anti-corrosion in metal surface chemistry, and metal clusters for catalysis. Also, from a new perspective of superatomic chemistry to cluster material genes [10], the insights into structural chemistry and reaction dynamics of metal clusters are anticipated to help for rational design of functional materials.

**Acknowledgements:** This work was supported by national Thousand Youth Talents Program, National Natural Science Foundation of China (Grant No. 21722308), and CAS Key Research Program of Frontier Sciences (CAS QYZDBSSWHL024).

## References

- [1] Z. Luo, A.W. Castleman, *Acc. Chem. Res.*, 47 2931-2940 (2014).
- [2] Z. Luo, A. W. Castleman, Jr. and S. N. Khanna, *Chem. Rev.*, 116, 14456-14492 (2016).
- [3] Z. Luo, S. Khanna, *Metal Clusters and Their Reactivity*, Springer, Springer Nature Singapore Pte Ltd., (2020).
- [4] B. Yin, Q. Du, L. Geng, H. Zhang, Z. Luo\*, S. Zhou\* and J. Zhao, *J. Phys. Chem. Lett.* 11, 5807-5814 (2020).
- [5] C. Cui, Y. Jia, H. Zhang, L. Geng and Z. Luo\*, *J. Phys. Chem. Lett.*, 11, 8222-8230 (2020).
- [6] H. Zhang, H. Wu, Y. Jia, B. Yin, L. Geng, Z. Luo\*, K. Hansen, *Commun. Chem.*, 3, 148 (2020).
- [7] Y. Jia, X. Yu, H. Zhang, L. Cheng, Z. Luo\*, *J. Phys. Chem. Lett.*, 12, 5115-5122 (2021).
- [8] L. Geng, M. Weng, C.-Q. Xu, H. Zhang, C. Cui, H. Wu, X. Chen, M. Hu, H. Lin, Z.-D. Sun, X. Wang, H.-S. Hu, J. Li, J. Zheng, Z. Luo\*, F. Pan\*, J. Yao\*, *Natl. Sci. Rev.*, 8, nwa201 (2021).
- [9] B. Yin, Q. Du, L. Geng, H. Zhang, Z. Luo\*, S. Zhou\*, J. Zhao, *CCS Chem.*, 3, 1-13 (2021).
- [10] B. Yin, Z. Luo\*, *Coord. Chem. Rev.*, 429 213643 (2021).

## 报告摘要

## 口头报告

## Photochemical Reaction Mechanism Studies on Selected Organic Molecular Systems

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Our research group focus on studying the photochemical reaction mechanisms on selected organic molecular systems, as well we investigated the photophysical process relating with the photocatalysts. State-of-art time-resolved spectroscopies of ultrafast transient absorption spectra and nanosecond time-resolved resonance Raman spectroscopy are utilized to directly detect the transient species and reactive intermediates involved in the photochemical reactions. As a strong support, DFT calculations are performed to simulate the UV-vis and Raman spectra and depict the reaction pathways.

Here, the work on the organic photochemical reaction mechanisms will be reported. First part is the photochemical reaction mechanism on aromatic carbonyl compounds in aqueous solutions<sup>5-10</sup>. The second part is the photodeprotection reaction mechanism studies on photolabile protecting groups<sup>11-16</sup>. The third part is the reaction mechanisms on the photoinduced quinone methide species<sup>17-20</sup>.

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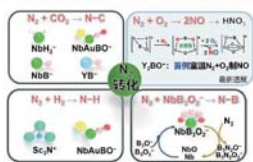
## References

## 报告摘要

## 口头报告

过渡金属离子团簇介导N<sub>2</sub>室温转化马嘉骥<sup>1</sup><sup>1</sup>北京理工大学, 化学与化工学院  
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氮气(N<sub>2</sub>)是最丰富廉价的氮源。但由于键能高(9.8 eV)、HOMO-LUMO gap大(10.8 eV),因此N<sub>2</sub>在室温下极稳定、难活化。而现在几乎人类使用的所有含氮化合物都以NH<sub>3</sub>为基本原料。目前工业上广泛采用的合成氨条件十分苛刻,需要350-500°C的高温,以及50-200atm的高压,全球合成氨所消耗的能源占全人类总能源消耗的1-2%<sup>[1]</sup>。实现温和条件下N<sub>2</sub>高效活化转化是一个极具挑战的课题。目前该过程的微观反应机理、活性调控方法及核心影响因素仍不十分清楚。在分子水平获得上述信息对于理解相关反应、设计催化剂具有重要意义。我们利用团簇模型构效关系清晰、可研究基元反应等优势开展研究,获得以下结果:1)在多金属活化N<sub>2</sub>的工作基础上,我们提出了利用单金属位点活化N<sub>2</sub>的新模式:金属-配体活化(Metal-Ligand Activation, MLA)模式<sup>[2]</sup>。利用p区主族元素代替一个或多个过渡金属,在与N<sub>2</sub>吸附、活化、转化过程中体现出高活性。MLA模式有利于N<sub>2</sub>被活化后的进一步转化过程。2)实现了N<sub>2</sub>和CO<sub>2</sub>室温下偶联形成N-C键<sup>[3,4]</sup>并实现了N<sub>2</sub>催化循环<sup>[5]</sup>。

图1: N<sub>2</sub>转化制N-C键、N-B键等示意图。

Acknowledgements: 基金委重大研究计划(91961122)

## References

- [1] Erisman, J. W.; Sutton, M. A.; Galloway, J.; Klimont, Z.; Winiwarter, W., *Nat. Geosci.* 2008, 1, 636-639.
- [2] Ding Y. Q.; Li Y.; Ying F.; Wang M.; Ma J. B., *J. Phys. Chem. Lett.* 2022, 13, 492-497.
- [3] Wang M.; Chu L. Y.; Li Z. Y.; Messinis Antonis M.; Ding Y. Q.; Hu L. R., Ma J. B., *J. Phys. Chem. Lett.* 2021, 12, 3490-3496.
- [4] Wang M.; Zhou H. Y.; Messinis Antonis M.; Chu L. Y.; Li Y.; Ma J. B., *J. Phys. Chem. Lett.* 2021, 12, 6319-6319.

## 报告摘要

## 口头报告

## Mapping partial wave dynamics in scattering resonances by low-energy NO-He collisions

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One of the most important parameters that determines the outcome of a collision is the 'miss-distance' or impact parameter, which in quantum mechanics is described by quantized partial waves. Here we present a joint experimental and theoretical study of low-energy NO-He collisions, that allows us to probe how individual partial waves evolve during the collision. By tuning the collision energies to scattering resonances between 0.2 and 8.5 cm<sup>-1</sup>, the initial conditions are characterized by a limited set of partial waves. We probed the lowest-lying resonance dominated by s and p waves only. The highly structured differential cross sections directly reflect the increasing number of contributing waves as the energy is increased.

By preparing NO in a rotationally excited state before the collision and by studying rotational de-excitation collisions, we were able to add one quantum of angular momentum to the system and trace how it evolves. Exploiting the principle of detailed balance, we show that rotational de-excitation collisions probe time-reversed excitation processes with superior energy and angular resolution. Our results are in good agreement with state-of-the-art quantum chemistry calculations at the CCSDT(Q) level.

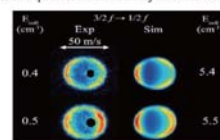


Figure 1: Experimental and simulated velocity map images at the collision energy of 0.4 cm<sup>-1</sup> for NO molecules scattered from  $j=3/2$  f state to  $j=1/2$  f state in NO-He collisions.

## References

- [1] T. de Jongh, M. Besemer, Q. Shuai, et al., *Science*, 368 626 (2020).
- [2] T. de Jongh, Q. Shuai, et al., *Nat. Chem.*, 14 538 (2022)

报告摘要

口头报告

过氧自由基的结构及反应动力学研究

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过氧自由基是大气化学反应中重要的中间体, 在复合污染形成过程中扮演着关键角色, 与大气氧化性、光化学臭氧和二次有机气溶胶的生成等密切相关。过氧自由基具有浓度低、种类多和结构复杂等特点, 其检测具有较大的技术挑战。本报告中, 我将介绍课题组在过氧自由基的结构及反应动力学研究方面的最新进展。采用流动管反应器和烟雾箱模拟大气氧化过程, 以真空紫外放电灯和同步辐射作为电离源, 结合自行研制的真空紫外光电离自由质谱仪, 在线检测获得了氧化过程中的反应物、产物和自由基等物种信息, 并开展了其反应动力学研究。通过测量光电离效率谱和光电子谱, 结合量子化学理论计算, 实现了过氧自由基同分异构体和转动构象体的检测, 以及自反应中二聚体产物的结构信息。

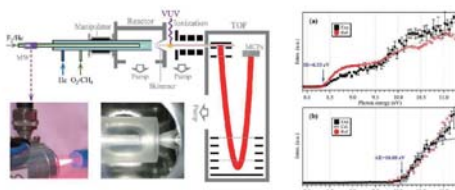


图1. 真空紫外光电离自由质谱, C<sub>2</sub>H和C<sub>2</sub>H<sub>2</sub>O:自由基的光电离效率谱。

References

- [1] X. Tang, X. Lin, G. A. Garcia, J.-C. Loison et al., Chem. Comm. 56, 15525 (2020)
- [2] Z. Wen, X. Tang, C. Fittschen, C. Zhang et al., Rev. Sci. Instrum. 91, 043201 (2020)
- [3] Z. Wen, X. Lin, X. Tang, B. Long et al., Phys. Chem. Chem. Phys. 23, 22096 (2021)
- [4] X. Lin, X. Tang, Z. Wen, B. Long et al., Atmos. Environ. 271, 118914, (2022)
- [5] F. L. Author, H.-G. Test, book title (publishing company, place, year).

报告摘要

口头报告

Aggregation induced spectral splitting theory and the inter-molecular & intramolecular interaction in binary mixture

Huigang Wang<sup>1,2</sup>, Xuming Zheng<sup>3</sup> and Yanying Zhao<sup>2</sup>

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The Aggregation Induced spectral Splitting theory (AIS) was proposed in view of the polarized Raman non-coincidence effect of polar molecules in binary mixture<sup>1</sup>. The relations between the symmetry of in-phase and out-phase stretching vibration, the depolarization ratio, the polarized vertical and parallel Raman components and the non-coincidence effect are established. Coexistence of intramolecular and intermolecular interaction in the binary mixture were analyzed from experimental data and schrodinger equations. It is expected to introduce new ideas for the study of intermolecular forces, aggregation research and molecular recognition.

Mode	Frequency (cm <sup>-1</sup> )	Intensity	Depolarization Ratio
ν <sub>1</sub>	1650	High	0.1
ν <sub>2</sub>	1600	Medium	0.2
ν <sub>3</sub>	1550	Low	0.3

Table 1 Summary of AIS model

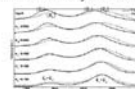


Fig 1 The VV and VH Raman components of vinylene carbonate/CH<sub>3</sub>CN mixtures

$$\begin{bmatrix} E_a^{(0)} - E & W & V & 0 \\ W & E_b^{(0)} - E & 0 & 0 \\ V & 0 & E_c^{(0)} - E & 0 \\ 0 & 0 & 0 & E_d^{(0)} - E \end{bmatrix} = 0$$

$$E_{1,2} = \frac{1}{2} (E_a^{(0)} + E_b^{(0)}) \pm \frac{1}{2} [X_0^2 + 4(V \pm W)^2]^{1/2}$$

$$E_{3,4} = \frac{1}{2} (E_c^{(0)} + E_d^{(0)}) - \frac{1}{2} [X_0^2 + 4(V \pm W)^2]^{1/2}$$

Four solution:  
Fig 2 four energies solutions to the schrodinger equation

**Acknowledgements:** This work was supported by National Natural Science Foundation of China(21873084) and Zhejiang Province Natural Science Foundation(LZ17B030001)

References

- [1] W. Xu, F. Wu, Y. Zhao, R. Zhou, H. Wang, X. Zheng, B. Ni, Scientific Reports 7 (2017) 43835.
- [2] Y. Han, R. Liu, C. Jiang, H. Wang, X. Zheng, Journal of Molecular Liquids 335 (2021) 116224 and 337 (2021) 116436...



## 报告摘要

## 口头报告

## Largescale Nonadiabatic Dynamics Methods and Applications

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In chemistry, physics, biology and material sciences, many important processes are relevant to nonadiabatic dynamics. While exact quantum dynamics simulations are limited to small systems and rate theories rely on certain perturbations, nowadays mixed quantum-classical dynamics becomes perhaps the only approach with the potential to simulate largescale nonadiabatic dynamics in complex systems. At energy degeneracy, however, the nonadiabatic coupling diverges and results in severe numerical instability. In fact, a single mistake in treating surface crossings could result in useless simulation results. In the past years, we have proposed a series of methods to solve this problem [1]. The time step size convergence has been greatly improved and a large time step size of about 1 fs can already achieve reliable simulations [2]. We consider an important subspace of adiabatic states for surface hopping, and size-independent results is rigorously obtained [3]. Using a subsystem to construct the electronic Hamiltonian, we significantly extend the nonadiabatic dynamics simulation to systems with hundreds of thousands states [4]. To study realistic systems, we propose a divide-and-conquer approach to construct the system Hamiltonian, which combines the advantages of Wannier analysis and machine learning. Real-time and real-space simulation of charge transport in coved graphene nanoribbons with over ten thousand atoms has been successfully realized and transient delocalization/localization is observed [5]. Especially, we have studied charge transfer dynamics across quantum dot/polymer interfaces, which implies the important roles of entropy and energetic disorders. This reveals that electron leakage is a key efficiency-loss channel in green and blue quantum dot light-emitting diodes and provides general strategies to improve the power-conversion efficiencies [6].

**Acknowledgements:** This work has the support of the National Natural Science Foundation of China (Grant Nos. 21922305 and 21873080).

## References

- [1] L. Wang, J. Qiu, X. Bai, J. Xu, WIREs Comput. Mol. Sci., 10 e1435 (2020).
- [2] J. Qiu, X. Bai, L. Wang, J. Phys. Chem. Lett., 9 4319 (2018).
- [3] J. Qiu, X. Bai, L. Wang, J. Phys. Chem. Lett., 10 637 (2019).
- [4] J. Qiu, Y. Lu, L. Wang, J. Chem. Theory Comput., 18 2803 (2022).
- [5] Z. Wang, J. Dong, J. Qiu, L. Wang, ACS Appl. Mater. Interfaces, 14 22929 (2022).
- [6] Y. Deng, F. Peng, Y. Lu, X. Zhu, W. Jin, J. Qiu, J. Dong, Y. Hao, D. Di, Y. Gao, T. Sun, M. Zhang, F. Liu, L. Wang, L. Ying, F. Huang, Y. Jin, Nat. Photonics, 16 505 (2022).

## 报告摘要

## 口头报告

H+HD(v=1, j=2)→H<sub>2</sub>+D 反应立体动力学实验研究王玉奉<sup>1</sup>, 杜天宇<sup>1</sup>, 王威<sup>1</sup>, 谢雨润<sup>2</sup>, 肖春雷<sup>1\*</sup>, 戴东旭<sup>1</sup>, 杨学明<sup>1,2\*</sup><sup>1</sup>分子反应动力学国家重点实验室, 大连化学物理研究所, 辽宁省大连市中山路457号<sup>2</sup>理学院, 南方科技大学, 广东省深圳市南山区学苑大道1088号

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立体动力学是反应动力学的重要分支, 着重研究化学反应中的方向性质, 例如不同方向反应物对于反应本身的影响。近年来, 立体动力学有着诸多进展<sup>[1-4]</sup>, 但是氢分子参与的化学反应的立体动力学仍是一片空白, 主要原因是氢分子的Raman激发截面很小, 很难获得高效率的激发。

针对这一难题, 我们发展了高功率的单纵模OPO/OPA光源<sup>[5]</sup>, 利用它对于氢分子进行受激拉曼泵浦(Stimulated Raman Pumping, SRP), 成功获得了足够高的激发效率。我们将这一技术与氢原子里德堡标记飞行时间谱方法结合, 并应用到交叉分子束实验中, 对于H+HD(v=1, j=2)→H<sub>2</sub>+D反应进行了立体动力学研究。通过控制SRP激光偏振, 我们控制HD分子键轴在反应中为三种碰撞构型: 平行、垂直、45°斜入, 进而研究不同构型对于该反应的影响。在0.5 eV、1.2 eV两个碰撞能下, 我们采集得到了不同构型下的微分散射截面, 发现该反应存在着很强的立体效应。

## References

- [1] Fengyan Wang, Kopin Liu, T. Peter Rakitzis. Nature Chemistry, 4, 636(2012).
- [2] Thomas R. Sharples et al. Nature Chemistry, 10, 1148(2018).
- [3] Cornelia G. Heid et al. Nature Chemistry, 11, 662(2019).
- [4] Haowen Zhou et al. Science, 374, 960(2021).
- [5] Yufeng Wang et al. Rev. Sci. Instrum., 91, 053001(2020).

## 报告摘要 口头报告

## Single Solvent Molecules Affect the Dynamics of Gas-Phase Ion-Molecule Nucleophilic Substitution Reactions

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Solvents have a profound influence on chemical reactions, and the  $S_N2$  nucleophilic substitution reaction,  $X + CH_3Y \rightarrow XCH_3 + Y^-$ , is a paradigm reaction in organic chemistry. Recent studies discovered the gas-phase ion-molecule  $S_N2$  reactions have complicated mechanisms and individual solvent molecules can affect their dynamics significantly. [1,2] Here, we first report a newly discovered  $S_N2$  mechanism, denoted as halogen-bonded complex mechanism, that initiates with front-side attack at halogen and end up with configuration inverted products. This mechanism becomes more important under singly-/doubly-hydrated condition. [3] Our direct dynamics simulation of singly hydrated peroxide ion reacting with  $CH_3Cl$  reveals a new product channel that forms  $CH_3OH + Cl^- + HOOH$ , besides the traditional channel that forms  $CH_3OOH + Cl^- + H_2O$ . This finding shows that singly hydrated peroxide ion behaves as a dual nucleophile through proton transfer between  $HOO^-$  ( $H_2O$ ) and  $HO^-$  ( $HOOH$ ). This study represents the first example of a single solvent molecule altering the nucleophile in a gas-phase ion-molecule  $S_N2$  reaction, signifying the importance of dynamical effects of solvent molecules. [4] We further investigate the generality of this phenomena and illustrate the nature of the competition as the degree of solvation increase. [5,6]

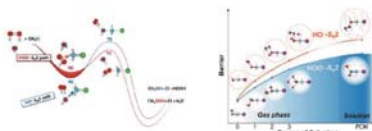


Figure 1: Potential energy profile (left) and barrier change (right) of competing  $HO^-/HOO^-$   $S_N2$  pathways of  $HOO^- (H_2O) + CH_3Y$  reaction.

**Acknowledgements:** This work has the support of National Natural Science Foundation of China (No. 21903004)

## References

- [1] J. Xie, W. L. Hase\*. Science, 352, 32-33 (2016)
- [2] R. Otto, J. Brox, R. Wester\* etc. Nat. Chem. 4, 534-538 (2012).
- [3] X. Ji, C. Zhao, J. Xie\* Phys. Chem. Chem. Phys. 23, 6349-6360 (2021)
- [4] C. Zhao, X. Wu, J. Xie\* etc. J. Phys. Chem. Lett., 12, 7134-7139 (2021)
- [5] X. Wu, C. Zhao; J. Xie\* ChemPhysChem, e202200285 (2022)
- [6] X. Ji, J. Xie\* Phys. Chem. Chem. Phys., 24, 7539 (2022).

## 报告摘要 口头报告

## Constructing Diabatic Potential Energy Matrices towards Dynamic Accuracy with Neural Networks Based on Adiabatic Energies and Physical Considerations

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Nonadiabatic reaction dynamics consecutively appears at frontiers of chemical reaction dynamics owing to the involvement of a wide variety of innovative issues such as nonadiabatic transition, geometric phase effect, nonadiabatic resonances, and quantum interferences. Our understanding of the nonadiabatic reaction dynamics largely relies on the diabatic potential energy matrix (PEM) of the system. However, it is often challenging to construct an accurate diabatic PEM of the system in practice due to the costly nonadiabatic couplings in *ab initio* calculations and the difficulties in the diabaticization methods for the diabatic PEM, especially for the molecular systems with strong nonadiabatic couplings manifested by conical intersections (CIs).

In this report, the new diabaticization methods by means of polynomials and neural networks (NNs) for the diabatic PEMs of the photoexcited molecules will be discussed, in which the diabaticization scheme is solely based on adiabatic energies without the associated costly derivative couplings. Taking the photodissociation of thiophenol for example, new diabatic PEMs near the CIs constructed by new methods were shown to well reproduce nonadiabatic attribute in terms of lifetime of the  $S_1$  vibronic states in contrast to available theoretical and experimental results. The good agreement validates the dynamic accuracy of the new PEMs by the NN approach. Furthermore, the new diabaticization procedure is shown to very efficient thanks to no need of the costly nonadiabatic couplings. Recently, we extended the diabaticization method that fits the diabatic PEM locally near the CIs to represent the diabatic PEM globally with additional physical considerations. The diabatic PEMs constructed by new methods for the photodissociation of  $H_2O$  via B band and  $NH_3$  via A band will be discussed.

## References

- [1] H. Song, C. Li, C. Xie, Phys. Rev. A 105, 022822 (2022).
- [2] S. Hou, C. Li, H. Han, C. Xie, Chin. J. Chem. Phys. 35, 461 (2022).
- [3] C. Li, S. Hou, C. Xie, Chin. J. Chem. Phys. 34, 825 (2021).
- [4] C. Li, C. Xie (in preparation).

## 报告摘要

## 口头报告

## Cleavage of the N≡N Triple Bond by borylene and Silylene

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A complete cleavage of the triple bond of N<sub>2</sub> by fluoroborylene (:BF) and silylenes (:SiH<sub>2</sub>) was achieved in a low-temperature N<sub>2</sub> matrix by the formation of the four-membered heterocycle FB(μ-N)<sub>2</sub>BF, which lacks a trans-annular NN bond. In addition the linear complex FB=NN=BF and cyclic FB(μ-N)<sub>2</sub> were formed. These novel species were characterized by their matrix-infrared spectra and quantum-chemical calculations. The puckered four-membered ring B<sub>2</sub>N<sub>2</sub> complex shows a delocalized aromatic 2-electron system in conjugation with the exo-cyclic fluorine π lone pairs. Similar works were also done by silylene (:SiH<sub>2</sub>). The four-membered heterocycle H<sub>2</sub>Si(μ-N)<sub>2</sub>SiH<sub>2</sub>, the silicon inserting molecule HNSiNH molecule formed by one silicon inserting HNNH and the end-on molecule H<sub>2</sub>SiNH were produced. This work may contribute to a rational design of catalysts for artificial dinitrogen activation.

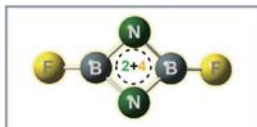


Figure 1: The four-membered heterocycle FB(μ-N)<sub>2</sub>BF show a complete cleavage of the nitrogen N<sub>2</sub> triple bond and a delocalized aromatic 2-electron bond conjugated with the exo-cyclic fluorine lone pairs.

**Acknowledgements:** This work has the support from the National Natural Science Foundation of China (nos. 21371136 and 21873070).

## References

- [1] B.Xu, X. Wang, etc, *Angew. Chem. Int. Ed.*, 60 17205 (2021).
- [2] B.Xu, X. Wang, etc, *Inorg. Chem.*, 58 2363 (2019).
- [3] B.Xu, X. Wang, etc, *Chem. Commun.* 57 2301 (2021).

## 报告摘要

## 口头报告

## Ultrafast Dynamics of Self-Trapped Excitons in Lead-Free Perovskite Nanocrystals

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Lead-free halide perovskite nanocrystals (NCs) have received increasing attention owing to their low toxicity and high stability. Strong carrier-phonon coupling in lead-free perovskite NCs facilitates the formation of self-trapped excitons (STEs), which typically give a broadband photoluminescence (PL) emission with a large Stokes shift. We highlight how PL modulations can give rise to an efficient white-light emission by understanding and tuning the ultrafast dynamics of STEs in lead-free perovskite NCs. We then present the exciton energy transfer mediated by STEs to provide an efficient thermally activated delayed fluorescence and dopant PL. We also illustrate promising directions for future applications based on STEs. We hope that this study can provide a new viewpoint for researchers to understand the ultrafast dynamics of STEs and promote lead-free perovskite NCs for optoelectronic applications.

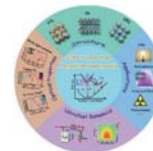


Figure 1: Self-trapped excitons in lead-free perovskite nanocrystals

## Acknowledgements:

This work has the support of the National Natural Science Foundation of China (Grant Nos. 21833009, 22005295).

## References

- [1] Yang, B.; Han, K\*.; *Acc. Chem. Res.* 2019, 52: 3188.
- [2] Liu, S.; Yang, B\*.; Han, K\*.; et al. *Angew. Chem. Int. Ed.* 2020, 59: 21925.
- [3] Kong, Q.; Yang, B\*.; Han, K\*.; et al. *Angew. Chem. Int. Ed.* DOI: 10.1002/anie.202105413.



## 报告摘要

## 口头报告

## Modulating photoexcited electronic process in molecular systems using chemical group modification

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Photoexcited electronic processes, such as intersystem crossing (ISC) and charge transfer (CT), are crucial for opto-electronic conversion, molecular luminescence and photochemical processes. We have conducted a series of first-principle study to explore how to modulate such processes in organic photo-responsive molecular systems using chemical group modification. First, chemical group modification of an organic fluorescent molecule with intrinsically small spin-orbit couplings could appreciably promote ISC rate by restraining the competing fluorescence rate. For N-substituted naphthalimides, selected electron donating groups (-OH, -OCH<sub>3</sub>) can alter the configuration of excited molecule, which turn the lowest singlet state from local excitation to charge transfer excitation and tilt the competition between fluorescence emission and ISC towards the latter.<sup>1</sup> Then, we found in the framework of Marcus theory that electron donating groups in pyrene-based photocatalyst can promote CT of  $\pi$ -stacked catalyst-reactant complexes while electron withdrawing groups have the opposite effect.<sup>2</sup> Second, we have developed a "donor-switch-acceptor" (D-S-A) model to demonstrate how the self-adaptive photoswitches can be used for restraining charge recombination in a donor-acceptor system. As an azobenzene is inserted between the donor and acceptor of a platinum(II) terpyridyl complex, its E $\rightarrow$ Z isomerization triggered by the photoexcited CT breaks the conjugation between donor and acceptor and turns off through-bond charge recombination.<sup>3</sup> Then, the idea of D-S-A is extended to dynamically control through-space charge transfer, which takes place as a donor-acceptor system with a co-facial or co-planar conformation via non-covalent interaction such as  $\pi$ -stacking or hydrogen bonding is photoexcited. The switchable bridged azobenzene adopts the compact Z conformation to facilitate through-space charge transfer between donor and acceptor, and then isomerizes to the extended E conformation to break non-covalent interaction between donor and acceptor and thus restrain charge recombination.<sup>4</sup> The concept of D-S-A suggests a simple way of modulating either through-bond or through-space charge transfer by incorporating a self-adaptive photoswitch moiety in the molecular design.

## Acknowledgements:

The above mentioned work has been supported by the National Key Research and Development Program of China and National Natural Science Foundation of China.

## References

- [1] Liu, R.; et al.; Zhang, G. J. Phys. Chem. Lett., 10 (2019) 1388.
- [2] Liu, R.; et al.; Zhang, G. J. Phys. Chem. Lett., 10 (2019) 3962.
- [3] Wu, Z.; et al.; Jiang, J. J. Phys. Chem. Lett. 9 (2018), 837.
- [4] Zhou, H; et al.; Zhang, G. J. Phys. Chem. Lett. 12 (2021) 3868.

## 报告摘要

## 口头报告

## 胰岛素二聚体的解离动力学研究与调控

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胰岛素是调控人体血糖的关键蛋白, 与糖尿病、阿尔茨海默等疾病的发病率密切相关。胰岛素在人体内以六聚体形式储存, 解离成单体后才具有血糖调节功能。因而, 寻找制约解离过程的特定氨基酸及中间态结构成为了调控胰岛素功能及研发新型类似物的关键。基于纳秒激光诱导的温度阶跃二维红外光谱系统 (T-jump 2D-IR), 对于探测生物大分子的细微结构变化、局域溶剂化等过程具有极好结构及时间分辨率。在此基础上, 针对氯化钙样品池诱导蛋白质聚合、热速率高等问题, 我们采用镀膜、延迟线降噪、欠采样等创新方法, 成功将时间窗口探测范围拓宽5倍至15毫秒。样品量降低4倍至6微升、探测效率提升2倍, 为探测热诱导下分子间的键价变化, 研究生物大分子的微环境和中间态结构提供了重要手段。通过引入最大熵模型进行瞬态光谱分析等方法完成了一系列胰岛素二聚体解离动力学的工作, 发现了二聚体的疏水核心是调控解离过程的关键, 并通过改变溶液环境实现了对该过程的调控。我们首次发现二甲亚砆可以通过疏水侧链的溶剂化过程促使二聚体解离, 乙醇在该作用基础上进一步破坏了内部的 $\alpha$ 螺旋结构, 而在纯水溶液中两个胰岛素单体可以在界面 $\beta$ 折叠被破坏的情况下, 通过疏水相互作用维持二聚体形态。通过结合马尔科夫状态模型和二维光谱模拟, 这些胰岛素的多种中间态结构得到了证实, 为新型胰岛素类似物的研发提供了重要依据。

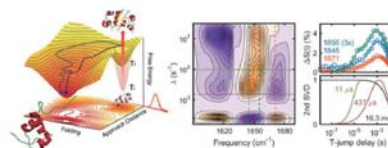


Figure 1: (left) schematic of insulin dimer dissociation induced by T-jump laser. (middle) The rate distribution of t-HDVE spectra analyzed with maximum entropy method. (top-right) Single-frequency kinetic traces at various frequency. (bottom-right) Amplitude components obtained with constrained single value decomposition analysis.

## References

- [1] Zhang, X.-X. and Tokmakoff, A., J. Phys. Chem. Lett., 11, 4353 (2020).
- [2] Zhang, X.-X.; Brantley S., etc., Commun. Biol., 3, 525 (2020).
- [3] Zhang, X.-X., Jones, K. C., etc., J. Phys. Chem. B, 120, 5134 (2016).



## 报告摘要

## 口头报告

## 量子态分辨的绝热和非绝热反应动力学理论研究

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量子反应动力学能够在量子态分辨的水平详细精确地研究一系列重要的基元化学反应。近来,这方面的研究已经取得了重大进展,发现了化学反应中普遍存在但很难被观测到的量子效应。这些进展一方面依赖于在实验中反应物分子量子态的精确制备和产物分子特定量子态的探测,另一方面离不开在理论上用精确的量子力学来描述分子中原子核的运动,这为研究分子反应动力学提供了最为精确的理论结果。在过去的一段时间里,我们致力于该领域的理论研究,开发了ABR程序包,用于研究非绝热反应动力学、态-态反应动力学,特别是发展了基于量子过渡态框架(QTS)的方法,发展了计算多原子体系微分散射截面的理论方法。具体地,我们使用全维高精度原子核量子动力学计算,详细研究了OH(A)+H<sub>2</sub>非绝热体系中的立体动力学,解决了理论-实验长期存在的一个分歧<sup>1</sup>;在量子过渡态框架下,通过引入态选择的热流算符,能够更加有效的研究过渡态对反应的控制<sup>2</sup>;在对H+CD<sub>3</sub>→HD+CD<sub>2</sub>反应的研究中,发现探测HD产物量子态比CD<sub>2</sub>产物量子态能够提供更高精度的测量结果<sup>3</sup>。

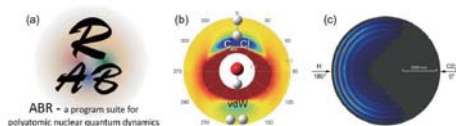


图 1. (a) ABR程序包; (b) H<sub>2</sub>+OH(A)非绝热反应中的立体动力学; (c) H+CD<sub>3</sub>→HD+CD<sub>2</sub>反应的微分散射截面。

## 参考文献:

- [1]. B. Zha, S. Han, C. Malbon, U. Manthe, D. R. Yarkony and H. Guo, Nat. Chem. 13, 909 (2021).
- [2]. B. Zhao, Phys. Chem. Chem. Phys. 23, 12105 (2021).
- [3]. B. Zhao, in preparation (2022).

## 报告摘要

## 口头报告

## High resolution laser spectroscopy of astrophysically relevant carbon-containing radicals

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About 200 molecules have been identified in the inter- and circumstellar medium, the highly dilute regions in between and around stars. Observations of these molecules provides excellent diagnostics of the physical conditions and chemical processes in the environments where they exist. In recent years, we have performed laboratory spectroscopic studies on astrophysically relevant small molecules, motivated to provide direct laboratory data needed to support and guide on-going and future observational missions in astrochemistry. A supersonically expanding planar plasma was employed to produce jet-cooled radicals and ions of astrophysical interest. Highly sensitive CRDS and/or LIF techniques were used to record the electronic transition spectra of transient species in the plasma. To achieve a high spectral resolution, we have also developed a nanosecond pulsed laser source with an output laser bandwidth close to the Fourier-transform limit. We have experimentally studied high resolution electronic spectra of small silicon and carbon cluster species (SiC<sub>n</sub>, Si<sub>2</sub>C<sub>n</sub>, etc.), potential precursors of interstellar carbonaceous dusts, and more recently, a series of resonance stabilized radicals (RSRs), such as vinylpropargyl, phenylpropargyl, heptatrienyl indenyl, and indanyl radicals, which are important intermediates in the formation of large polycyclic aromatic hydrocarbons (PAHs). The resulting laboratory data are supportive for the optical observations of the diffuse and translucent interstellar clouds, and also stand on its own for a comprehensive understanding of the intrinsic molecular properties.

## 报告摘要

## 口头报告

## Investigation of Photophysical Mechanism of Organic Aggregates by Multiscale Modeling

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## Abstract:

Organic aggregates are universal in nature. The luminescent mechanism of organic aggregates are complex and are highly dependent on the molecular packing, intermolecular interactions and excited state process. Therefore it is a big challenge in study the photophysical properties of complex organic aggregates. To unravel the relationship between the assembled organic aggregates and the luminescent properties, we performed systematic study of assembled organic aggregates with different degree of order (from amorphous aggregates, ordered host-guest complexes, highly ordered biological systems) by multiscale modeling protocol, combining the thermal vibration correlation function based excited state decay rate formalism,

we found that the assembled organic aggregates blocks the excited-state nonradiative decay channels by suppression of electron-vibration coupling and enhancing the fluorescent intensity. In addition, we proposed at the first time that the linear relationship between the fluorescent intensity and size of amorphous aggregates, and then proposing the charge controlled strategy for design fluorescent probe to selectively target specific organelles.



## References

1. Xiaoyan Zheng\*, Dong Wang\*, Wenhan Xu, Siqin Cao, Qian Peng\*, Ben Zhong Tang\*. Materials Horizons, 2019, 6, 2016-2023.
2. Xiaoyan Zheng, Lizhe Zhu, Xiangze Zeng, Luming Meng, Lu Zhang, Dong Wang, Xuhui Huang\*. The Journal of Physical Chemistry Letters, 2017, 8(8): 1798.
3. Junfang Yang, Qian Peng, Ruide Xue, Zesheng Li, Xiaoyan Zheng\*. Materials Chemistry Frontiers, 2021, 5: 1806-1816.
4. Yi Zeng, Junfang Yang, Xiaoyan Zheng\*. Physical Chemistry Chemical Physics, 2021, 23(41): 23986-23997.

## 报告摘要

## 口头报告

d-d Transition Mediated Electron Transfer at Acetone/-TiO<sub>2</sub>(110) Interface

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Interfacial charge transfer is crucial in solar to chemical and electrical energy conversion. Here, we report an electron transfer to the adsorbed acetone layers mediated by d-d transition within TiO<sub>2</sub> substrate. An excited state at -E<sub>r</sub>+2.1 eV on acetone covered TiO<sub>2</sub>(110) has been detected by two-photon photoemission spectroscopy (2PPE). According to photon energy-, polarization-, substrate orientation- and surface reduction-dependent measurements, this new excited state is attributed to an acetone adlayer related state which is populated via d-d transition in the TiO<sub>2</sub> octahedron with the long axis along [110]<sup>1,2</sup>. The origin of the excited state is discussed.

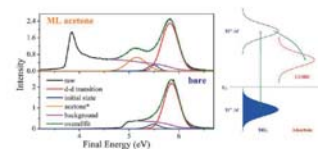


Figure 1: Comparative 2PPE spectra from bare and 1 monolayer acetone covered TiO<sub>2</sub>(110) and schematic of electron transfer at acetone/TiO<sub>2</sub> interface.

**Acknowledgements:** This work was supported by the National Natural Science Foundation of China (21973092) and the National Key Research and Development Program of China (2021YFA1500601 and 2018YFA0208703).

## References

- [1] Yang et al, J Am Chem Soc, 137, 9146 (2015).
- [2] Zhou et al, J Phys Chem Lett, 12, 10515 (2021).

## 报告摘要

## 口头报告

## Coherent Vibrational Dynamics of Metal Clusters

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Probing the coherent vibrational dynamics of gold nanoclusters is of great importance to understand their electron-vibration interactions and optical properties. As the size of gold nanocluster increases, the evolution from discrete electronic state to continuous band can also be reflected in their coherent vibrational dynamics. In metal nanoparticles with continuous band, laser pulses will heat them can initiate vibration and periodic shift of surface plasmon resonance band, which causes oscillations in their excited state population dynamics. In molecular-like metal nanoclusters, laser pulse will lead to single electron transition and initiate coherence between electronic and vibrational states, which causes periodic modulations on excited states. We have observed significant coherent vibrational dynamics of several different-sized gold nanoclusters using ultrafast transient absorption spectroscopy. Frequency and phase analysis on these oscillations can help assigning the origin of these coherent oscillations. Detailed study on these coherent vibrational dynamics will help to further understand these nanoclusters in the transition size regime.

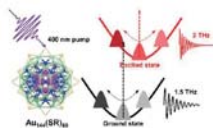


Figure 1: Coherent Vibrational Dynamics of  $Au_{144}(SR)_{46}$  nanoclusters

**Acknowledgements:** This work has the support of Chinese Academy of Sciences (YSBR-007)

## References

- [1] Zhang, W.; Kong, J.; Li, Y.; Kuang, Z.; Wang, H.; Zhou, M., *Chem. Sci.* 2022, 13, 8124-8130.
- [2] Kong, J.; Wu, Y.; Zhou, M., *Chin. J. Chem. Phys.* 2021, 34, 598-604.
- [3] Zhou, M.; Du, X.; Wang, H.; Jin, R., *ACS Nano* 2021, 15, 13980-13992.5330-5336 (2016).

## 报告摘要

## 口头报告

## Neural Network Based MD Simulation Reveals Detailed Complex Reaction Processes in Combustion

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Atomic-level understanding of complex combustion processes is of significant importance in chemistry and related industries. Here, a neural network-based molecular dynamics (MD) approach is developed to simulate the combustion process of methane in real time. Through MD simulation, detailed reaction processes leading to the creation of combustion products and various intermediate molecular species are intimately revealed and characterized, with a total of 798 different chemical reactions being recorded from a single MD trajectory. Our approach is as accurate as the ab initio MD simulation but far more efficient in computation. The present work heralds the dawn of a new era in which MD simulations of complex reaction systems at ab initio level can be routinely carried out to complement or even replace some laboratory experiments.

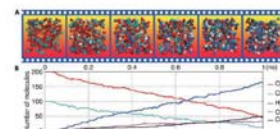


Fig. 1 Real-time dynamics of methane combustion.

**Acknowledgements:** This work was supported by the National Natural Science Foundation of China (grant nos. 91641116).

## References

- [1] Zeng, J.; Cao, L.; Chin, C. H.; Ren, H.; Zhang, J. Z. H.; Zhu, T., *Phys. Chem. Chem. Phys.*, 22, 683, (2020).
- [2] Zeng, J.; Cao, L.; Xu, M.; Zhu, T.; Zhang, J. Z., *Nat. Commun.* 11, 5713, (2020).
- [3] Zeng, J.; Zhang, L.; Wang, H.; Zhu, T., *Energy & Fuels* 21, 762, (2021).
- [4] Xiao, J.; Zhang, J.Z.H.; Zhu, T., to be submitted.
- [2] F. L. Author, H.-G. Test, book title (publishing company, place, year).

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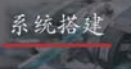
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