人工智能浪潮下超快光谱研究的挑战与机遇

When Ultrafast Spectroscopy Meets AI: Challenges and Opportunities

网址：

http://ias.ust.hk/events/202512ufsai/home.php

会议手册

2025年12月05日至2025年12月08日

香港科技大学化学系

非常感谢各位老师出席“人工智能浪潮下超快光谱研究的挑战与机遇”研讨会，并做报告。本次会议将于2025年12月5日至8日在中国香港特别行政区九龙清水湾的香港科技大学举行，由香港科技大学化学系和香港城市大学物理系联合承办。

一. 组织机构

主办单位：
中国香港特别行政区九龙清水湾香港科技大学化学系

承办单位：
香港科技大学化学系，香港城市大学物理系，香港科技大学赛马会高等研究院

大会主席：
杨学明院士、张东辉院士、周鸣飞教授

大会秘书长：
翁羽翔教授

大会执行秘书：
陈藤藤教授、张哲东教授

组委会：

陈藤藤，	香港科技大学
张哲东，	香港城市大学
黄晋卿，	香港科技大学
潘　鼎，	香港科技大学
万晴云，	香港中文大学
李海星，	香港城市大学

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二. 大会主旨

本次研讨会旨在汇聚超快光谱及相关交叉学科领域的顶尖专家，共同探讨**人工智能与超快光谱技术的深度融合及其在化学、材料、能源、物理和生命科学等领域的前沿应用与发展趋势，促进香港与内地的学术交流和融合**。会议将围绕以下议题展开深入讨论：

- **超快光谱在化学与材料科学中的应用**
- **人工智能在物质科学中的应用**
- **下一代超快光谱方法与技术**
- **超快光谱与人工智能的交叉融合**

我们非常荣幸地邀请到**杨学明院士**（中科院大连化物所），**张东辉院士**（中科院大连化物所）和**周鸣飞教授**（复旦大学，国家杰青）担任大会主席。届时，多位来自国内外知名机构的杰出科学家（如**香港大学的任咏华院士、美国科学院院士 Martin Zanni，清华大学李隽院士**等）将出席本次会议并作精彩学术交流。

三.会场信息

会场位于中国香港特别行政区九龙清水湾香港科技大学主校区，到达方式可以坐高铁到香港西九龙高铁站，随后打出租车到达香港科技大学北门（红鸟广场回旋处），出租车费大约港币现金200元，也可以用支付宝或者微信支付。或者坐飞机到达香港国际机场，在机场打出租车到达香港科技大学北门（红鸟广场回旋处），出租车费大约港币现金400元，也可以同样支付宝或者微信支付。

四. 注册相关信息

本次会议注册费收费标准为教师：人民币1000.00元，学生及博士后免除注册费，会议费用缴纳后，原则上不予退费。本次会议食宿费自理，组委会提供预订房间服务。

注册费收款方式为银行转账，转账信息如下：

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五. 学术报告准备细则

本次会议交流语言为尽量英文（如不擅长英文，中文交流也可以），准备报告 ppt 或幻灯片时要求内容采用英文，请提前了解您的报告时间，严格按照报告手册上的时间作报告（大会报告为30分钟+5分钟答疑时间，邀请报告为17分钟+3分钟答疑时间），会场地点在香港科技大学学术楼主楼 LT-D 和 LT-E 报告厅，报告具体安排以会议手册为准。

六. 用餐安排

	午餐	晚餐
12月05日		校内餐厅
12月06日	校内 UniBistro&Bar 西餐厅	维港游，海上自助餐厅
12月07日	校内南北小厨餐厅	西贡区洪记海鲜酒楼
12月08日		

七. 会议咨询

您在参会中遇到任何问题均可以选择咨询身边志愿者。

会后财务及发票信息咨询请联系组委会:

陈藤藤:tengtengchen@ust.hk， 张哲东： zzhan26@cityu.edu.hk

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY | DEPARTMENT OF CHEMISTRY

CityU Department of Physics
香港城市大學
City University of Hong Kong

八．赞助商

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY | IAS HKUST JOCKEY CLUB INSTITUTE FOR ADVANCED STUDY

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY | School of Science 理學院

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY | DEPARTMENT OF CHEMISTRY

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会议日程

日期/时间 (Date/Time)	**具体活动(Activities)**	**地点(Location)**
第一日 (2025年12月05日)		
14:00-21:00	会议注册(Registration)	主会场：学术楼主楼 LT-D 报告厅 (LT-D academic main building)
第二日(2025年12月06日)		
9:00-9:10	开幕式致辞(Opening Remarks)	主会场：学术楼主楼 LT-D 报告厅(LT-D)
9:10-9:20	集体合照(Group Photo)	(LT-D)
9:20-9:55	Plenary Talk 1: Are exciton dynamics in thin films representative of actual solar cells? Addressing the question using artifact-free ultrafast 2D photocurrent spectroscopy, **Prof. Martin T. Zanni,** University of Wisconsin, Madison	(LT-D)
9:55-10:30	Plenary Talk 2: Toward a Rational Understanding of Polariton Chemistry, **Prof. Wei Xiong,** University of California, San Diego	(LT-D)
10:30-10:50	Refreshments	主会场 LT-D 外(Outside LT-D)
10:50-11:25	Plenary Talk 3: Chemical Insight of Robotic AI-Chemist Based on Spectroscopic Descriptors, **Prof. Jun Jiang（江俊）** University of Science and Technology of China	(LT-D)
11:25-12:00	Plenary Talk 4: Quantum-state resolved mechanisms for complex reactions based on fundamental-invariant neural network potential energy surfaces, **Prof. Bina Fu（傅碧娜）** Dalian Institute of Chemical Physics, CAS	(LT-D)
12:00-14:00	午餐及休息时间(Lunch Time)	香港科技大学校园内 UniBistro & Bar 半自助午餐(Semi-Buffet at UniBistro&Bar)
分会场一(Section 1)		
14:00-18:00	**分会场一(Section 1)**	**学术楼主楼 LT-D 报告厅(LT-D)**
14:00-14:20	Invited Talk: Open system quantum dynamics and spectroscopy in molecular systems with strong light-matter coupling, **Prof. Qiang Shi（史强）** Institute of Chemistry, CAS	LT-D
14:20-14:40	Invited Talk: Photoexcitation Dynamics in Condensed-Phase Materials, **Prof. Run Long（龙闰）** Beijing Normal University	LT-D

日期/时间 (Date/Time)	具体活动(Activities)	地点(Location)
14:40-15:00	Invited Talk: Excited State Chirality Revealed by Ultrafast Time-resolved Chiral Spectroscopy, **Prof. Jinquan Chen（陈缙泉）** East China Normal University	LT-D
15:00-15:20	Invited Talk: Multi-State Density Functional Theory for Ground and Excited States, **Prof. Yangyi Lu（陆扬懿）** Shenzhen Bay Laboratory	LT-D
15:20-15:40	Invited Talk: Time-resolved dynamics of metal halide perovskite under high pressure, **Prof. Kaijun Yuan（袁开军）** Dalian Institute of Chemical Physics, CAS	LT-D
15:40-16:00	Invited Talk: Ultrafast scattering & spectroscopy study on a photoinduced thermochemical reaction, **Prof. Jie Yang（杨杰）** Tsinghua University	LT-D
16:00-16:20	**茶歇(Refreshment)**	**报告厅外(Outside LT-D)**
16:20-16:40	Invited Talk: What is the redox state of a dual function CraCRY? **Prof. Dongping Zhong（仲冬平）** Shanghai Jiaotong University	LT-D
16:40-17:00	Invited Talk: Excited State Dynamics of Metal Nanoclusters, **Prof. Meng Zhou（周蒙）** University of Science and Technology of China	LT-D
17:00-17:20	Invited Talk: Two-Dimensional Electronic Spectroscopy at 100 kHz Repetition Rate for Ultrafast Dynamics Study, **Prof. Jinhui Zhong（钟锦辉）** Southern University of Science and Technology	LT-D
17:20-17:40	Invited Talk: Exciton Delocalization and Transport in Layered Semiconductors, **Prof. Long Yuan（袁龙）** University of Science and Technology of China	LT-D
17:40-18:00	Invited Talk: Nonlinear optical spectroscopy of oxide/water interfaces, **Prof. Weitao Liu（刘韡韬）** Fudan University	LT-D
分会场二(Section II)		
14:00-18:00	**分会场二(Section II)**	**学术楼主楼 LT-E 报告厅(LT-E)**
14:00-14:20	Invited Talk: Out of the Blue: Discovery and Application of a Blue Fluorescent Amino Acid, **Prof. Feng Gai（盖锋）** Peking University,	LT-E
14:20-14:40	Invited Talk: Title Construction of Chemical Reaction Networks Driven by Both AI and Physics, **Prof. Tong Zhu（朱通）** East China Normal University	LT-E

日期/时间 (Date/Time)	具体活动(Activities)	地点(Location)
14:40-15:00	Invited Talk: Quantum mechanical deconstruction of energy transfer pathways modified by vibrational strong coupling, **Prof. Qi Yu（郁琦）** Fudan University	LT-E
15:00-15:20	Invited Talk: Algorithm-Driven Robotic Discovery of Polyoxometalate-Based Metal-Organic Frameworks, **Prof. Donglin He（贺冬琳）** The Hong Kong University of Science and Technology-Guangzhou	LT-E
15:20-15:40	Invited Talk: Phase-sensitive time-domain coherent techniques in nonlinear 2DES and ESFG spectroscopy, **Prof. Donghai Li（李东海）** University of Science and Technology of China	LT-E
15:40-16:00	Invited Talk: Memory Kernel Coupling Theory for Spin-Phonon Interactions in Molecular Qubits, **Prof. Wenjie Dou（窦文杰）** Westlake University	LT-E
16:00-16:20	**茶歇(Refreshment)**	**报告厅外(Outside LT-D)**
16:20-16:40	Invited Talk: Understanding Ultrafast Spin Dynamics in Halide Perovskites, **Prof. Xihan Chen（陈熹翰）** Southern University of Science and Technology	LT-E
16:40-17:00	Invited Talk: Spin Manipulation and Coherence Transfer of Colloidal Nanoplatelets, **Prof. Junhui Wang（王俊慧）** Dalian Institute of Chemical Physics, CAS	LT-E
17:00-17:20	Invited Talk: Ultrafast Vibrational Signatures of Conformationally Gated Phase Separation in a Natural Folded Enzyme, **Prof. Xiao You（尤晓）** Westlake University	LT-E
17:20-17:40	Invited Talk: Nonlinear Spectroscopic Studies on the Molecular Structure and Dynamics of Self-Assembly at Biological Interfaces, **Prof. Zhen Zhang（张贞）** Institute of Chemistry, CAS	LT-E
17:40-18:00	Invited Talk: Anion Recognition Investigated by Linear and Nonlinear Vibrational Spectroscopy, **Prof. Hongtao Bian（边红涛）** Shaanxi Normal University	LT-E
集体活动(Group Activity)		
18:30	**乘坐大巴去北角码头(Bus Shuttle to North Port)**	
19:30-21:45	**维港游，“幻彩咏香港”海上自助晚餐(Cruise Tour to Victoria Bay)**	北角码头， 有专车接送

日期/时间 (Date/Time)	具体活动(Activities)	地点(Location)
第三日(2025年12月07日)		
分会场一(Section I)		
8:30-11:50	**分会场一(Section I)**	**学术楼主楼 LT-D 报告厅(LT-D)**
8:30-8:50	Invited Talk: Ultrafast 2D IR Spectroscopy: Uncovering Hidden Structures and Dynamics in Proteins and Peptides, **Prof. Jianping Wang（王建平）** Institute of Chemistry, CAS	LT-D
8:50-9:10	Invited Talk: Remote Molecular Modulation in Polariton Chemistry, **Prof. Bo Xiang（项博）** Westlake University	LT-D
9:10-9:30	Invited Talk: Spatiotemporal Imaging of Ultrafast Carrier Dynamics in Optoelectronic Materials, **Prof. Wenming Tian（田文明）** Dalian Institute of Chemical Physics, CAS	LT-D
9:30-9:50	Invited Talk: Femtosecond Broadband Transient Fluorescence Spectroscopy, **Prof. Hailong Chen（陈海龙）** Institute of Physics, CAS	LT-D
9:50-10:10	Invited Talk: Ultrafast charge carrier dynamics in metal halide perovskites by Terahertz spectroscopy, **Prof. Heng Zhang（张恒）** Xiamen University	LT-D
10:10-10:30	**茶歇(Refreshments)**	**报告厅外(Outside LT-D)**
10:30-10:50	Invited Talk: A Multi-Agent System for Complex Chemical Reaction Information Extraction, **Prof. Hanyu Gao（高寒宇）** The Hong Kong University of Science and Technology	LT-D
10:50-11:10	Invited Talk: TBD, **Prof. Wenkai Zhang（张文凯）** Beijing Normal University	LT-D
11:10-11:30	Invited Talk: Soap Film Artificial Photosynthesis, **Prof. Hongwei Song（宋宏伟）** South China University of Science and Technology	LT-D
11:30-11:50	Invited Talk: Probing the Kinetics and Energetics of Charge Transfer States in Organic Bulk Heterojunctions, **Prof. Jiaying Wu（吴佳莹）** The Hong Kong University of Science and Technology-Guangzhou	LT-D
分会场二(Section II)		
8:30-11:50	**分会场二(Section II)**	**学术楼 LT-E 报告厅(LT-E)**

日期/时间 (Date/Time)	**具体活动(Activities)**	**地点(Location)**
8:30-8:50	Invited Talk: Detection and Regulation of Excited State Dynamics of Long Afterglow Room-Temperature Phosphorescence, **Prof. Ming-De Li（李明德）** Shantou University	LT-E
8:50-9:10	Invited Talk: TBD, **Prof. Guoqing Zhang（张国庆）** University of Science and Technology of China	LT-E
9:10-9:30	Invited Talk: Post-OPA Enhanced SFG Spectroscopy and Transient Absorption Microscopy, **Prof. Zefeng Ren（任泽峰）** Dalian Institute of Chemical Physics, CAS	LT-E
9:30-9:50	Invited Talk: Reaction Mechanisms on Selected Photocages, **Prof. Jiani Ma（马佳妮）** Shaanxi Normal University	LT-E
9:50-10:10	Invited Talk: Photoinduced charge transfer dynamics in the condensed phase, **Prof. Xiang Sun（孙翔）** New York University Shanghai	LT-E
10:10-10:30	**茶歇(Refreshments)**	**报告厅外(Outside LT-D)**
10:30-10:50	Invited Talk: Structure and Ultrafast Vibrational Dynamics of Interfacial Water at Polar Hydrophobic and Chiral Interfaces, **Prof. Shuji Ye（叶树集）** University of Science and Technology of China	LT-E
10:50-11:10	Invited Talk: Mechanism of aggregation-induced emission and control of excited state dynamics, **Prof. Junrong Zheng（郑俊荣）** Peking University	LT-E
11:10-11:30	Invited Talk: Reaction and Structural Dynamics in the Blue-Light Photoreceptors, **Prof. Bei Ding（丁蓓）** Shanghai Jiaotong University	LT-E
11:30-11:50	Invited Talk: Regulation and Application of Exciton Kinetics in Colloidal Quantum Dots, **Dr. Shan He（何山）** The Hong Kong University of Science and Technology	LT-E
12:00-14:00	**午餐及休息(Lunch)**	**香港科技大学学术楼南北小厨餐厅(G/F China Garden)**
14:00-14:20	Invited Talk: Multi-Modal Ultrafast Nonlinear (Vibrational) Spectroscopy for AI Future, **Prof. Hongfei Wang（王鸿飞）** Westlake University	学术楼主楼 LT-D 报告厅(LT-D)
14:20-14:40	Invited Talk: TBD, **Prof. Chunfeng Zhang（张春峰）** Nanjing University	LT-D

日期/时间 (Date/Time)	**具体活动(Activities)**	**地点(Location)**
14:40-15:00	Invited Talk: TBD, **Prof. Andong Xia（夏安东）** Beijing University of Posts and Telecommunications	LT-D
15:00-15:20	Invited Talk: Coherent energy transfer in photosynthesis revealed by two-dimensional electronic spectroscopy, **Prof. Yuxiang Weng（翁羽翔）** Institute of Physics, CAS	LT-D
15:20-15:40	Invited Talk: Nonadiabatic Dynamics of Ultrafast Intersite Charge Transfer during Chemical Bond Formation: Hydrogen Scattering from a Semiconductor Surface, **Prof. Bin Jiang（蒋彬）** University of Science and Technology of China	LT-D
15:40-16:00	**茶歇(Refreshments)**	**报告厅外(Outside LT-D)**
16:00-16:20	Invited Talk: Simulating spectroscopy and ultrafast dynamics in strongly correlated systems, **Prof. Haibo Ma（马海波）** Shandong University	LT-D
16:20-16:40	Invited Talk: Site-specific Functionality Tuning the Excited-State Dynamics of Thio-nucleobases, **Prof. Hongmei Su（苏红梅）** Beijing Normal University	LT-D
16:40-17:00	Invited Talk: Simulating Coherent Spin Dynamics of Surface Molecules, **Prof. Xiao Zheng（郑晓）** Fudan University	LT-D
17:00-17:15	大连创锐光谱	LT-D
17:15-17:20	闭幕式(Closing Ceremony)	LT-D
18:30-20:00	晚宴(Dinner)	香港西贡区洪记海鲜酒楼(Sai Kung Hung Kee Seafood)
第四日(2025年12月08日)		
参会代表自行离港(Departure)		

目前已确定参加的专家学者名单：

Name	Affiliation
1. Vivian Yam（任咏华）	The University of Hong Kong (HKU)（香港大学）
2. Jun Li（李隽）	Tsinghua University（清华大学）
3. Mingfei Zhou（周鸣飞）	Fudan University（复旦大学）
4. David Lee Philips	The University of Hong Kong (HKU)（香港大學）
5. Martin Zanni	University of Wisconsin- Madison
6. Wei Xiong	University of California, San Diego
7. Shuji Ye（叶树集）	USTC（中国科学技术大学）
8. Jun Jiang（江俊）	USTC（中国科学技术大学）
9. Bin Jiang（蒋彬）	USTC（中国科学技术大学）
10. Meng Zhou（周蒙）	USTC（中国科学技术大学）
11. Long Yuan（袁龙）	USTC（中国科学技术大学）
12. Donghai Li（李东海）	USTC（中国科学技术大学）
13. Guoqing Zhang（张国庆）	USTC（中国科学技术大学）
14. Chunfeng Zhang（张春峰）	Nanjing University（南京大学）
15. Dongping Zhong（仲冬平）	Shanghai Jiaotong University（上海交通大学）
16. Chang Yan（严畅）	Shanghai Jiaotong University（上海交通大学）
17. Bei Ding（丁蓓）	Shanghai Jiaotong University（上海交通大学）
18. Xiaodan Cao（曹潇丹）	Shanghai Jiaotong University（上海交通大学）
19. Qi Yu（郁琦）	Fudan University（复旦大学）
20. Weitao Liu（刘韡韬）	Fudan University（复旦大学）
21. Xiao Zheng（郑晓）	Fudan University（复旦大学）
22. Jinquan Chen（陈缙泉）	East China Normal University（华东师范大学）
23. Tong Zhu（朱通）	East China Normal University（华东师范大学）
24. Xiang Sun（孙翔）	New York University Shanghai（上海纽约大学）
25. Yuxiang Weng（翁羽翔）	Institute of Physics, CAS（中科院物理所）
26. Hailong Chen（陈海龙）	Institute of Physics, CAS（中科院物理所）
27. Jie Yang（杨杰）	Tsinghua University（清华大学）
28. Hanshi Hu（胡憾石）	Tsinghua University（清华大学）
29. Feng Gai（盖锋）	Peking University（北京大学）
30. Junrong Zheng（郑俊荣）	Peking University（北京大学）
31. Jianping Wang（王建平）	Institute of Chemistry, CAS（中科院化学所）
32. Qiang Shi（史强）	Institute of Chemistry, CAS（中科院化学所）
33. Zhen Zhang（张贞）	Institute of Chemistry, CAS（中科院化学所）
34. Andong Xia（夏安东）	Beijing University of Posts and Telecommunications（北京邮电大学）
35. Hongmei Su（苏红梅）	Beijing Normal University（北京师范大学）
36. Wenkai Zhang（张文凯）	Beijing Normal University（北京师范大学）
37. Long Run（龙闰）	Beijing Normal University (北京师范大学)
38. Yangyi Lu（陆扬懿）	Shenzhen Bay Laboratory（深圳湾实验室）
39. Hongfei Wang（王鸿飞）	Westlake University（西湖大学）
40. Wenjie Dou（窦文杰）	Westlake University（西湖大学）
41. Xiao You（尤晓）	Westlake University（西湖大学）
42. Bo Xiang（项博）	Westlake University（西湖大学）
43. Haibo Ma（马海波）	Shandong University（山东大学）
44. Kaijun Yuan（袁开军）	DICP, CAS（中科院大连化物所）
45. Zefeng Ren（任泽峰）	DICP, CAS（中科院大连化物所）
46. Junhui Wang（王俊慧）	DICP, CAS（中科院大连化物所）
47. Bina Fu（傅碧娜）	DICP, CAS（中科院大连化物所）
48. Wenming Tian（田文明）	DICP, CAS（中科院大连化物所）
49. Xihan Chen（陈熹翰）	Southern University of Science and Technology（南方科技大学）
50. Jinhui Zhong（钟锦辉）	Southern University of Science and Technology（南方科技大学）

51. Hongwei Song（宋宏伟）	South China University of Technology（华南理工大学）
52. Jiani Ma（马佳妮）	Shaanxi Normal University（陕西师范大学）
53. Hongtao Bian（边红涛）	Shaanxi Normal University（陕西师范大学）
54. Mingde Li（李明德）	Shantou University（汕头大学）
55. Heng Zhang（张恒）	Xiamen University（厦门大学）
56. Jiaying Wu（吴佳莹）	HKUST-GZ（香港科技大学（广州））
57. Donglin He（贺冬琳）	HKUST-GZ（香港科技大学（广州））
58. Hanyu Gao（高寒宇）	The Hong Kong University of Science and Technology（香港科技大学）
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60. Jinqing Huang（黄晋卿）	The Hong Kong University of Science and Technology（香港科技大学）
61. Hui Cao（曹晖）	The Hong Kong University of Science and Technology（香港科技大学）
62. Jue Wang （王珏）	The Hong Kong University of Science and Technology（香港科技大学）
63. Haipeng Lu（吕海鹏）	The Hong Kong University of Science and Technology（香港科技大学）
64. Yuxing Yao（姚昱星）	The Hong Kong University of Science and Technology（香港科技大学）
65. Shensheng Chen（陈伸升）	The Hong Kong University of Science and Technology（香港科技大学）
66. Tianlong Zhang（张天隆）	The Hong Kong University of Science and Technology（香港科技大学）
67. Shan He（何山）	The Hong Kong University of Science and Technology（香港科技大学）
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69. Tengteng Chen（陈藤藤）	The Hong Kong University of Science and Technology（香港科技大学）
70. Haixing Li（李海星）	City University of Hong Kong（香港城市大学）
71. Zhedong Zhang（张哲东）	City University of Hong Kong（香港城市大学）
72. Qingyun Wan（万晴云）	The Chinese University of Hong Kong（香港中文大学）
73. Hairong Lyu（吕海荣）	The Chinese University of Hong Kong（香港中文大学）

会议摘要：

Chemical Insight of Robotic AI-Chemist Based on Spectroscopic Descriptors

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Keywords: autonomous robotic platforms; iterative experimental feedback loop; spectroscopic intelligence; Robotic AI-Chemist

Abstract: Autonomous robotic platforms are fundamentally transforming chemical discovery paradigm, shifting from human-driven trial-and-error approach to high-throughput, closed-loop autonomous discovery. Central to platform autonomy lies the requirement for rich and unbiased data to guide iterative experimental feedback loop. Spectral data provide an ideal solution, serving as unified chemical descriptors that are inherently measurable, calculable, interpretable, and describable, correlating diverse chemical structures to their complex properties. This Perspective reviews the emerging field of spectroscopic intelligence, as well as how these spectroscopic descriptors empower the Robotic AI-Chemist. We first introduce the establishment of structure-spectrum-property AI models and the completion of missing property or function data based on spectroscopic descriptors. Then, we discuss how spectroscopic intelligence can bring new insights into chemical processes such as catalytic reactions and protein folding, and how it facilitates the closed-loop operation and inverse design capabilities essential for on-demand chemical generation. Lastly, we outline the synergistic future of integrating spectroscopic intelligence with large language models and Robotic AI-Chemist platforms. This Perspective aims to offer an outlook on the indispensable role of spectroscopy in driving Robotic AI-Chemists to achieve autonomous chemical discovery, accelerate intelligent screening, and advance complex inverse design.

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Are exciton dynamics in thin films representative of actual solar cells? Addressing the question using artifact-free ultrafast 2D photocurrent spectroscopy

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Keywords: Ultrafast Spectroscopy, Photovoltaic, Solar Cell

Abstract: The performance of many photoactive devices is impacted by the dynamics of excitons within the photoactive layer. Typically, these dynamics are deduced by independently conducted transient absorption measurements on films outside of the device with the assumption that the photophysics in free standing films inform the photophysics of the film inside the device. But there are interfaces in devices that are not present in films and the morphology and atomic packing might be impacted by device construction. Moreover, photoabsorption experiments measure all excitons whereas the best photovoltaic devices are perhaps 20% efficient, meaning that only 1 in 5 excitons actually produce electricity. Thus, the conclusions drawn from free standing films might not be directly relevant to devices. This talk will cover results made possible by new advances in ultrafast 2D photocurrent spectroscopy that enable ultrafast exciton dynamics to be directly compared between films and devices. In photovoltaics made from semiconducting carbon nanotubes, we find that the conclusions drawn from films versus devices are quite different, leading us to reinterpret long standing experiments and reevaluate our goals for device architecture.

References

1. ZM Faitz, D Im, CJ Blackwell, MS Arnold, MT Zanni, A spectrometer design that eliminates incoherent mixing signals in 2D action spectroscopies, J. Chem. Physics 161 (13), 2025
2. ZM Faitz, CJ Blackwell, D Im, A Dhavamani, M Arnold, MT Zanni Ultrafast photocurrent detection reveals that device efficiency is dominated by ultrafast exciton dissociation not exciton diffusion. arXiv preprint arXiv:2506.21402. 2025

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Quantum-state resolved mechanisms for complex reactions based on fundamental-invariant neural network potential energy surfaces

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Keywords: Roaming dynamics, FI-NN, complex reactions, excited state

Quantum state-resolved complex molecular dynamics theory is crucial for understanding phenomena in fields such as interstellar atmospheres and combustion chemistry. However, due to limitations in theoretical methods, high-precision, quantum state-resolved dynamics studies were traditionally confined to systems with low electronic states and a few atoms. We have developed an efficient and accurate Fundamental Invariant-Neural Network (FI-NN) potential energy surface construction method, which has advanced quantum state-resolved dynamics research to reaction systems involving more than 10 atoms. Through excited-state potential energy surface construction and quantum state-resolved dynamics methods, combined with experimental collaboration, we discovered the first roaming pathway in molecular high-excited-state dissociation, offering a new perspective for understanding and predicting photochemical reactions. Furthermore, we identified unique collision-induced roaming mechanisms in complex molecular reactions, providing theoretical insights for the development and refinement of theoretical models.

References

Y. Hao, B. Fu*, Dong H. Zhang, J. Chem. Theory Comput., 2025, 21, 1046.
Y. Bai, Y. Fu, B. Fu* et al, Nat. Commun, 2025, 16, 2732.
B. Fu*, W. Dong*, D. H. Zhang*, X. Yang* et al, Nat. Chem., 2025, 17, 897.

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Toward a Rational Understanding of Polariton Chemistry

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Keywords: Polaritons, Strong Coupling, 2D IR

Abstract: Mid-Infrared (MIR) light can interact with molecules by selectively exciting molecular vibrational modes. In combination with photonic structures, MIR can target specific vibrational states of molecular to influence chemical reactions. In this talk, I will explain how photonic environments can modify molecular dynamics through strong light-matter coupling. This strong coupling leads to the molecular vibrational polaritons – a hybrid quasiparticle between light and matter. Using two-dimensional infrared (2D IR) spectroscopy, we have demonstrated that strong coupling to photonic environments can efficiently promote energy transfer within or between molecules, subsequently slowing down competing reaction pathways. We further explored the criteria to fulfill polariton-enabled energy transfer, by which we discovered and verified a new principle to enable intermolecular energy transfer through polaritons in disorder materials. This research progress provide insights into a rational mechanism and designing photonic structures to modify chemical landscapes and influence reaction pathways.

References

1. Yin G., Liu T., Zhang L., Sheng T., Mao H., Xiong W., *Science*, 2025, Vol. 389, p.845
2. Liu T., Yin G., *Chemical Science*. 2025, Vol. 16, 4676.

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Coherent energy transfer in photosynthesis revealed by two-dimensional electronic spectroscopy

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Keywords: 2DES, coherent energy transfer, photosynthesis

The concept of quantum coherence is derived from the superposition principle in quantum mechanics. The advent of ultrashort laser pulse having a broad band spectrum can easily create superposition of a number of excited states undergoing quantum coherence. For photosynthetic light-harvesting complexes, coherent energy transfer is expected to have a higher efficiency than the classical pathway, while elucidating the nature of the coherence, i.e., electronic, electronic-vibtrational coupling and vibrational, is still challenging. Two-dimensional electronic spectroscopy (2DES) is a powerful tool in elucidating the coherent energy transfer, exciton delocalization and many other coherent processes In this talk，I will briefly introduce the principle and implementation of 2DES, and then report the recent progresses in exploring biological quantum effects either by using 2DES in our group: (1) quantum phase synchronization via electronic-vibronic energy dissipation sustains long-lived coherence to support coherent energy transfer in allophycocyanin (APC) trimer which is a photosynthetic light-harvesting pigment-protein complex located in the phycobilisomes (PC) of cyanobacteria and red algae; (2) Classical energy transfer in PC620, a main light harvesting antenna in the PC rod with its structure being very similar to that of APC; (3) Electronic-vibrational coherence in cryptophyte phycoerythrin 545 (PE545) antenna.

References

1. Zhu, R. et al., *Nature Communications*, 2024, 15, 3171.
2. Wang, J. et al., *J. Chem. Phys.* 2024, 161, 085101.
3. Wang, J. et al., *J. Chem. Phys.* 2025,205101.

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Structure and Ultrafast Vibrational Dynamics of Interfacial Water at Polar Hydrophobic and Chiral Interfaces

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Keywords: hydrophobic water layer; water monomers; chiral water; ultrafast vibrational dynamics; sum frequency generation vibration spectroscopy

Abstract: Interfacial water layers at polymer and biomolecular boundaries play a critical role in governing protein and biomolecular stability, dynamics, and function. Elucidating the structure and ultrafast dynamics of this confined water is therefore key to understanding the hydration mechanisms driving fundamental biological processes. Here, we report our investigations into the structure and ultrafast vibrational dynamics of water at fluorinated polymer and chiral biomolecule interfaces using femtosecond time-resolved sum frequency generation vibrational spectroscopy. Our studies have revealed a two-dimensional "hydrophobic water layer" on Teflon at room temperature [1], isolated "H_2O" monomers and chiral $OH^-(H_2O)$ species in Teflon matrices [2], and uncovered a structured "chiral water" arrangement at chiral interfaces [3]. This chiral water exhibits strong coupling to N-H vibrational modes while decoupling from achiral interfacial and bulk water, revealing its distinct behavior. Our findings highlight the pivotal role of chiral water in vibrational energy redistribution and propagation in biomolecular systems, and offer novel insights into chirality generation and transfer.

References

[1] Zhang, J. H.; Tan, J. J.; Pei, R. Q; Ye, S. J.; Luo, Y. *J. Am. Chem. Soc.* **2021**, *143*, 13074–13081.

[2] Zhang, J. H.; Pei, R. Q; Tan, J. J.; Ni, Z.J.; Ye, S. J.; Luo, Y. *J. Am. Chem. Soc.* **2023**, *145*, 26925–26931.

[3] Pei, R.Q.; Wang, M.M.; Chen, F.X.; Lai, J.; Tan, J.J.; Luo, Y.; Ye, S.J. *J. Am. Chem. Soc.* **2025**, 147, 36162–36169.

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Site-specific Functionality Tuning the Excited-State Dynamics of Thio-nucleobases

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A small chemical modification of the nucleobase structure can significantly enhance the photoactivity of DNA, which may incur DNA damage, thus holding promising applications in photochemotherapy treatment of cancers or pathogens. Thio-nucleobases due to the substitution of carbonyl oxo group by thio group are a representative category. Compared to the canonical nucleobases, the thiobases display unique photophysical and photochemical properties. Their primary absorption spectra are red-shifted to the UVB (280 – 315 nm) and UVA (315 – 400 nm) region, and the sulfur substitution dramatically increases the rate of intersystem crossing (ISC) to the triplet manifold. To furnish guidance on photochemical applications of thiobases, we have been performing studies of 6-methylthioguanine (me6-TG), 5-Phenylethynyl-4-thiouridine (5ph-4TU), and 2-Thiocytosine (2tCyt) etc. by femtosecond and nanosecond time-resolved spectroscopy with high-level *ab initio* calculations, disentangling the site-specific functionality tuning effect on the excited state dynamics.

For example, in me6-TG, we find that the double substitution (thionation and methylation) boosts the photoactivity by introducing more reactive channels. Intriguingly, $^1n_N\pi^*$, rather than $^1n_S\pi^*$, acts as the doorway state engendering the formation of the long-lived reactive triplet state. The $^1n_N\pi^*$ induces a low spin-orbit coupling of 8.3 cm^{-1}, which increases the intersystem crossing (ISC) time (2.91±0.14 ns). Despite of the slowed ISC, the triplet quantum yield (Φ_T) still accounts for a large fraction (0.6±0.1), consistent with the potential energy surface that favors excited state bifurcation to $^1n_N\pi^*_{min}$ (3.36±0.15 ps) rather than $^1\pi\pi^*_{min}$ (5.05±0.26 ps), such that the subsequent ISC to triplet via $^1n_N\pi^*_{min}$ constitutes the main relaxation pathway. Moreover, the effect of thionation in synergy with methylation opens a unique C-S bond cleavage pathway through crossing to a repulsive $^1\pi\sigma^*$ state, generating thiyl radicals as highly reactive intermediates that may invoke biological damage. This photodissociation channel is extremely difficult for conventional nucleobases. Our findings demonstrate the synergistic effects of double functionality substitution in modulating excited state dynamics and enhancing the photolabile character of DNA nucleobases, providing inspirations for the rational design of advanced photodynamic and photochemotherapy approaches.

References

[1] Q Zhou, Y Hao, J Jie, S Wang, Y Xia, C Yang, L Liu, W Fang, H Su, *JACS Au*, **2024**, *4*, 441

[2] C Yang, F Wang, Q Zhou, J Jie, H Su, *J. Phys. Chem. Lett.*, **2023**, *14*, 10585

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Simulating Coherent Spin Dynamics of Surface Molecules

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Keywords: spin dynamics, electron spin resonance, surface molecule, open quantum system, quantum dissipation

Abstract: Surface magnetic molecular systems hold broad application prospects in cutting-edge fields such as quantum sensing, quantum computing, and surface catalysis. However, the many-body correlation effects inherent in these systems, coupled with the complex influence of the surface environment on molecular spin states, pose significant challenges for theoretical simulation. Furthermore, recent advancements in experimental techniques have expanded the manipulation of molecular spin states on surfaces from quasi-static to coherent dynamic control. To echo the challenges posed by these latest experiments, we develop high-precision quantum statistical dynamics methods to accurately characterize the influence of the environment on molecular spin states [1]. By continuously enhancing the precision and "resolution" of our first-principles-based approaches, we have been able to accurately reproduce a series of experimental observations [2,3]. This presentation will highlight specific examples to demonstrate the productive interplay between new experiments and novel theories in recent years, while also offering perspectives on future development trends in related fields.

References

[1] D. Zhang, L. Ye, J. Cao, Y. Wang, R.-X. Xu, X. Zheng, and Y.J. Yan, *WIREs Comput. Mol. Sci.* **14**, e1727 (2024).
[2] L. Ye, X. Zheng, and X. Xu, *Phys. Rev. Lett.* **133**, 176201 (2024).
[3] X. Ding, J. Cao, X. Zheng, and L. Ye, *J. Chem. Phys.* 162, 084114 (2025).

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Quantum mechanical deconstruction of energy transfer pathways modified by vibrational strong coupling

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Keywords: Polariton, Vibrational spectrum, Energy transfer

Abstract: Polariton chemistry has become a rapidly growing field, offering new possibilities for manipulating chemical properties by coupling molecular systems with the electromagnetic field of an optical cavity. This talk focuses on how vibrational strong coupling (VSC) within the cavity influences molecular spectra and vibrational energy transfer processes. I will briefly present the development of the cavity VSCF/VCI method, enabling accurate linear and nonlinear vibrational spectra of molecules-cavity hybrid systems. Then taking $(H_2O)_{21}$-cavity as an example, I will introduce the combination of cavity VSCF/VCI method, quantum wavepacket dynamics and accurate machine learning potential to resolve underlying mechanisms of energy transfer under VSC. I will also demonstrate how the collective VSC promotes the delocalization of OH stretches, and opens new intermolecular vibrational energy pathways involving both neighboring and remote water molecules.

References

[1] Yu, Q.*; Zhang, D.H.; Bowman, J.M. *Nat. Commun.* 2025, 16, 6760

[2] Yu, Q.*; Bowman, J.M. *J. Chem. Theory Comput.* 2024, 20, 4278

[3] Yu, Q.*; Bowman, J.M. *Nat. Commun.* 2023, 14, 3527

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Soap Film Artificial Photosynthesis

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The world's energy demand of 15 trillion Watts is expected to double by 2050. We need clean energy and a potential solution is the sun. The best way to store solar energy is through fuels which are1-2 orders of magnitude more energy dense than the best batteries (that are also environmentally more hazardous). **Artificial Photosynthesis (AP)** represents a scheme for capturing and storing the vast energy from sunlight in chemical bonds of a solar fuel while liberating O2 as by-product. We propose a technology paradigm shift through this responsible research & innovation project, aimed at developing renewable solar fuel production, exploiting the unique self-assembling property of surfactants, and proton transport properties in soap films. We have designed the concept of an economic artificial photosynthetic membrane in form of stable soap film with engineered photocatalytic surfaces, formed at the junction between a dissymmetric soap bubble pair. We have developed novel lipid photocatalysts; have demonstrated AP within liposomes (micro-analogues of soap bubbles in an aqueous environment), and charge dissymmetric bubble junction stability, which are critical conditions for project plausibility.

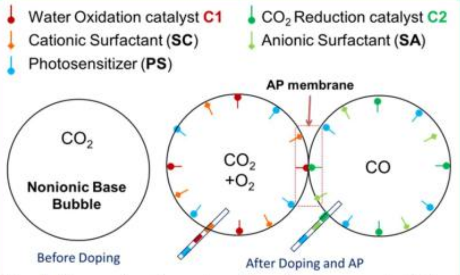

Fig 1 Concept schematic of nonionic soap bubbles doped with functional surfactants - **specifically at their inner surfaces**. A photosynthetic membrane will be formed at their junction generating CO & O_2 from CO_2, water and light.

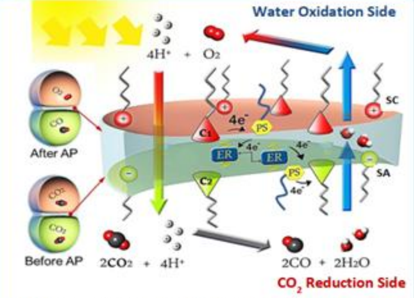

Fig 2 Cross-section of soap film based AP membrane formed at the junction of a dissymmetric bubble pair. **C1**: Water oxidation catalyst; **C2**: CO_2 reduction catalyst; **ER**: Electron relay; **PS**: Photosensitizer. Blue arrows represent H_2O molecules moving through film to oxidation side. Red-Green arrow represents H^+ transport to reduction side.

References：

[1] Phys. Rev. Lett. 132, 028201 (2024)

[2] J. Am. Chem. Soc. 2022, 144, 21, 9399–9412

[3] J. Am. Chem. Soc. 2022, 144, 42, 19353–19364

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Excited State Chirality Revealed by Ultrafast Time-resolved Chiral Spectroscopy

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Keywords: Excited state chirality, ultrafast dynamics

Abstract: Chirality is one of the universal phenomena in nature. Research on the mechanisms governing the generation, transmission, amplification, and regulation of molecular chirality is currently evolving from traditional macroscopic steady-state investigations to emerging microscopic transient-level studies. To address this, we have developed ultrafast time-resolved chiral spectroscopic techniques and analytical methods, establishing a technical foundation for elucidating the origin and evolution mechanisms of excited-state chirality in molecular systems. By using the femtosecond time-resolved circular dichroism (fs-TRCD) and femtosecond-nanosecond circularly polarized luminescence (TR-CPL) spectroscopy technologies, we achieved simultaneous analysis of molecular excited-state dynamics and the generation/evolution processes of excited-state chirality. This revealed the mechanisms by which picosecond-scale excited-state chirality in molecular and supramolecular systems cooperatively evolves through intersystem crossing, electron spin polarization, and energy transfer. Finally, focusing on the structure-activity relationship between DNA chiral secondary structures and their triplet excited states/photochemical properties, we designed and constructed a series of DNA-targeting photosensitizer molecules based on excited-state chiral engineering. This work unveils their reaction mechanisms in biological chiral environments.

References

1. Wang, X.; Wu, P.; Wang, Y.; Cui, T.; Jia, M.; He, X.; Wang, W.; Pan, H.; Sun, Z.; Yang, H-B.; Chen, J.*; Angew. Chem. Int. Ed. 2024, 64, e202407929.

2. Cui, Y.; Ai, J.; Duan, Y.; Jia, M.; Ouyang, T.; Liu, A.; Yu, L.; Liu, J.; Liu, X.; Chu, C.; Li, Y.; Ma, Y.; Chen, L.; Han, L.*; Chen, J.*; Tian, C.*; Che, S.*; Fang, Y.* ; Chem, 2025, 11: 102390

3. Han, Y.; Yang, X.; Wang, X.; Mao, H.; Huang, K.; Pan, H.; Liu, M.; Duan, P.*; Chen, J.*; J. Am. Chem. Soc., 2025, 147, 9891-9899.

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Nonlinear Spectroscopic Studies on the Molecular Structure and Dynamics of Self-Assembly at Biological Interfaces

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Keywords: Nonlinear spectroscopy; Interfacial molecular structure; Self-assembly; High-resolution sum frequency generation spectroscopy;

This study investigated the molecular-scale interactions of amino acids and homopolypeptides with phospholipid membranes by integrating high-resolution sum-frequency generation vibrational spectroscopy (SFG-VS) with thermodynamic analysis and molecular dynamics (MD) simulations. We probed the real-time structural changes induced by five natural amino acids and four polypeptides in phosphatidylcholine monolayers, monitoring key functional groups (e.g., methyl, methylene, carbonyl, phosphate), while MD simulations clarified the corresponding assembly sites and binding modes. Our results demonstrate that the binding affinity of amino acids is governed by their distinct chemical properties, whereas polypeptide binding efficiency is co-determined by side chain structure, hydrogen-bonding capacity, and overall chemical character. These findings reveal fundamentally different membrane-binding mechanisms between amino acids and peptides, providing insights into primordial molecular processes. Furthermore, this work provides a molecular-scale basis for the rational design of drug delivery systems. Future studies will explore chiral molecular assembly mechanisms and ultrafast dynamics at cell membrane interfaces.

References

[1] Zhang, Y.; Qin, X.; Zhu, X.; Liu, M.; Guo, Y.; Zhang, Z*., Nat Commun 2022, 13 (1), 7737.
[2] Yu, C.; Shang, P.; Guo, Y.; Zhang, Z.,.J Phys. Chem. B. B 2024, 128 (8), 1892-1899.

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Ultrafast 2D IR Spectroscopy: Uncovering Hidden Structures and Dynamics in Proteins and Peptides

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Keywords: 2D IR; Membrane protein; Chemical exchange

Abstract: This presentation highlights the application of ultrafast two-dimensional infrared (2D IR) spectroscopy to resolve site-specific structural and dynamic features in complex biological systems. In the first study, using uniformly ^{13}C,^{15}N-labeled lysine residues in bacteriorhodopsin, we identified a high-frequency amide-I mode at ~1693 cm^{-1} assigned to K159. This residue forms a structured γ-turn with E161 on the cytoplasmic surface, stabilizing the E–F loop and facilitating proton uptake. Complementing this, the second study investigates hydration dynamics near a β-peptide backbone using *N*-ethylpropionamide in D_2O. Two distinct amide-I sub-bands reveal dynamically exchanging strongly and weakly hydrogen-bonded water states, with sub-picosecond exchange kinetics and an activation energy of ~13 kJ/mol. Together, these works demonstrate how 2D IR spectroscopy, combined with isotopic labeling and computations, can unveil transient conformations and hydration dynamics critical to protein function, offering a powerful approach for studying large biomolecules in native-like environments.

References

1. Rong Hu, Xiaoyan Ding, Pengyun Yu, Xuemei He, Anthony Watts, Xin Zhao, and Jianping Wang, *J. Am. Chem. Soc.* **2022**, *144*, 22083-22092.
2. Juan Zhao, Pengyun Yu, Tiantian Dong, Yanzhou Wu, Fan Yang, and Jianping Wang, *Commun. Chem.* **2024**, 7, 82.

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Phase-sensitive time-domain coherent techniques in nonlinear 2DES and ESFG spectroscopy

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Keywords: Phase-sensitive nonlinear detection; Two-dimensional electronic spectroscopy; Electronic sum-frequency-generation spectroscopy

Since their development, nonlinear spectroscopic techniques have greatly expanded our ability to interrogate microscopic structures and ultrafast dynamics in materials. In practical studies, the detected signals often originate from the coherent superposition of multiple nonlinear contributions. For instance, two-dimensional (2D) spectroscopy typically requires isolating and distinguishing signals associated with different Liouville pathways, while sum-frequency-generation (SFG) spectroscopy often demands separating signal components originating from distinct interfaces or even from the bulk. As a result, the phase of a nonlinear signal becomes crucial as complementary information beyond its intensity.

Heterodyne detection is a widely used approach for retrieving phase information in nonlinear spectroscopy; however, its implementation generally involves complex optical architectures, thereby raising the experimental barrier. Here, we introduce a 2D spectroscopy method based on shot-to-shot phase cycling [1] and a SFG spectroscopy approach employing time-domain ptychography [2]. Both techniques achieve phase-sensitive nonlinear detection through time-domain scanning while preserving relatively simple optical layouts that do not require heterodyne detection. The incorporation of artificial intelligence–driven spectral acquisition and analysis is expected to further enhance the capabilities of these methods.

References

[1] Xinyu Zhao, Donghai Li*, *J. Chem. Phys*. 2025, 163, 114202.
[2] Pengyun Yu, Donghai Li*, *Opt. Express* 2025, 33, 40157.

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Understanding Ultrafast Spin Dynamics in Halide Perovskites

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Keywords: Spin polarized Lifetime, Ultrafast spin dynamics

Abstract: The development of an efficient and stable energy conversion system requires a mechanistic understanding of the energy conversion process in different materials. Hybrid perovskite material systems show extraordinary promise in the field of optoelectronics in spin applications due to dynamic Rashba splitting. Although previous work has identified important contributions from the dynamic structural response, the proposed lattice-carrier coupling mechanism is not yet fully understood. In this talk, we report small polaron formation (short-range electron-phonon interactions) in (4AMP)PbI4, where we directly visualize strong electron-phonon coupling via coherent acoustic phonon signals. At the same time, the deformation potential analysis could be further expanded to understand spin dynamics at high carrier density in (3AMP)PbI4, as well as carrier scattering potential in thermoelectric materials. Finally, to fully understand the factors governing the spin-relaxation in perovskites, a machine learning algorithm is developed and adopted to establish a HOMO-LUMO and polarizability-based spin relaxation rate. With the deep level of understanding of spin dynamics, the full photophysical and photochemical process can be resolved.

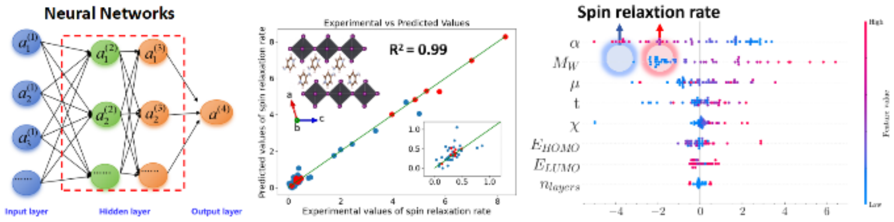

Fig. 1 Machine learning Framework for spin polarized dynamics

References

[1] Huang, Y.; **Chen, X.*** *J. Am. Chem. Soc.*, 2024, 146: 12225-12232

[2] Li, J.; **Chen, X.*** *Chem. Sci.*, 2025, DOI: 10.1039/D5SC07406A

[3] Huang, Y.; **Chen, X.*** *Natl. Sci. Rev.*, 2025, nwae461

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Memory Kernel Coupling Theory for Spin-Phonon Interactions in Molecular Qubits

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Keywords: Spin-phonon interactions, Molecular qubits, memory kernel

Abstract: Dynamical observables are often described by time correlation functions (TCFs). However, efficiently computing TCFs for complex quantum systems remains a significant challenge, as it typically requires solving the full dynamical evolution of the system. In this work, we propose the memory kernel coupling theory (MKCT)—a general theoretical framework for calculating TCFs. This approach builds upon the memory kernel formalism established by Mori and avoid the calculation of projected dynamics by further decomposing the memory kernel into auxiliary kernel functions. As a result, only steady state moments are required to obtain the TCFs, which greatly simplify the calculation of quantum dynamics in complex systems. This general framework is numerically validated on typical open quantum systems, namely the spin-boson model and the Anderson impurity model. Furthermore, we apply it to systems with nonlinear environment coupling, obtaining accurate dynamical and spectral properties. Finally, we employ MKCT to study the spin-phonon relaxation process in a molecular qubit. The numerical results successfully explain novel spin relaxation phenomena observed in experiments.

References

1. W. Liu, Y. Su, Y. Wang, W. Dou. Phys. Rev. Lett. 135, 148001 (2025).
2. R. Bi, Y. Su, Y. Wang, L. Sun, W. Dou. J. Chem. Phys. 161, 024105 (2024).

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Simulating spectroscopy and ultrafast dynamics in strongly correlated systems

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Keywords: strongly correlated systems; quantum chemistry; vibronic dynamics; X-ray absorption spectroscopy; attosecond electron dynamics

Abstract: Recent years have witnessed significant breakthroughs in the field of excited-state chemistry experiments. In terms of characterization techniques, advancements in experimental methods-such as extreme ultraviolet light sources, ultrafast spectroscopy, and ultra-high-resolution electron microscopy—have enabled scientists to achieve precise observation of excited states with atomic spatial resolution on femtosecond to attosecond timescales. Regarding the dimensionality of research systems, innovations in molecular design and synthesis, along with external field control techniques, have progressively expanded the scope of study from small gas-phase molecules to multi-scale systems, including aggregates and complex photoelectric environments. However, as system complexity continues to increase, a number of theoretical challenges have become increasingly prominent. These include quantum many-body strong correlation effects, relativistic effects in heavy elements, non-adiabatic effects, strong light-matter coupling, and multi-scale computational issues. This report will introduce our electronic structure and dynamics methods for strongly correlated systems, developed based on the density matrix renormalization group (DMRG), along with their demonstrative applications in areas such as electronic spectroscopy, anharmonic vibrational spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, X-ray absorption spectroscopy, femtosecond non-adiabatic dynamics, and attosecond electron dynamics.

References

1. Cheng Y., Ma H., *J. Chem. Theory Comput.* 2024, 20, 1988.
2. Xu Y., Liu C., Ma H., *J. Chem. Phys.* 2024, 161, 052501.
3. Sun X., Ma H., *J. Chem. Phys.* 2025, 163, 164115.

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Probing the Kinetics and Energetics of Charge Transfer States in Organic Bulk Heterojunctions

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Organic bulk heterojunctions (BHJs) have emerged as promising candidates for photovoltaic and photocatalytic applications due to their tunable electronic properties and low-cost fabrication. However, a comprehensive understanding of the ultrafast charge dynamics within these complex systems is essential to optimize their performance for solar to energy conversion. In this talk, I will present our recent investigations using pump-push-probe spectroscopy to understand the charge separation and recombination processes in organic BHJs designed for optoelectronic applications. This advanced spectroscopic technique allows us to explore the higher excited states and transient intermediates that play a critical role in charge carrier dynamics. Our studies provide critical insights into the mechanisms of charge generation and transfer at the donor-acceptor interface, highlighting the influence of molecular architecture and energy landscape. By employing a push pulse, we selectively perturb the system to access states beyond the initial photoexcitation, providing a deeper understanding of how energy is redistributed and how the system returns to equilibrium and how systems evolve beyond the initial excitation and understanding pathways that lead to different photophysical or photochemical outcomes.

Keywords:

Abstract: ultrafast charge carrier dynamics, pump-push-probe spectroscopy, donor/acceptor interface, charge generation and transfer, higher excited states

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Detection and Regulation of Excited State Dynamics of Long Afterglow Room-Temperature Phosphorescence

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Keywords: Room temperature phosphorescence; Excited state; energy transfer; intersystem crossing

Abstract: The host-guest doping strategy is a rapidly developing method for preparing room-temperature phosphorescence (RTP) materials in recent years. It has advantages such as simple preparation, low cost, diverse molecular structures, and controllable performance. Doping systems can regulate different lifetimes and colors of RTP by adjusting the electronic structure between host and guest molecules, achieving long afterglow materials with excellent performance. However, the mechanism of intersystem crossing enhancement in host-guest doped long afterglow material systems remains unclear, making it rather difficult to regulate their optical properties. Therefore, conducting theoretical calculations on the host-guest doped long afterglow RTP materials, exploring their luminescent mechanism and regulation strategy, is an urgent problem to be solved in the RTP. Here, we have studied donor/acceptor molecules with different electronic energy levels through theoretical calculations, ultrafast transient absorption, and fluorescence spectroscopy, to detect the lifetime of the charge/energy transfer processes and screen out suitable donor or acceptor molecules. The excited state relaxation process of RTP is revealed. Ultimately, intelligent manufacturing of high-performance organic long afterglow RTP materials would be fabricated.[1-3]

References

[1] Li, J.; Hao, S.; Li, M.; Chen, Y.; Li, H.; Wu, S.; Yang, S.; Dang, L*.; Su, S. J*.; **Li, M. D***. *Angew. Chem. Int. Ed.* **2024**, 63, e202417426.

[2] Yang, G.; Hao, S.; Deng, X.; Song, X.; Hyun, W. J.; **Li, M. D***.; Dang, L*. Nat. Commun. 2024, *15*, 4674.

[3] Yang, G.; Li, J.; Deng, X.; Song, X.; Lu, M.; Zhu, Y.; Yu, Z.; Xu, B.; **Li, M. D***.; Dang, L*. *J. Phys. Chem. Lett.* 2023, *14*, 6927–6934.

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Spatiotemporal Imaging of Ultrafast Carrier Dynamics in Optoelectronic Materials

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Keywords: carrier dynamics, pressure, photoelectric conversion, optoelectronics devices

Abstract: The efficiency of photoelectric conversion is fundamentally governed by the dynamics of photogenerated charge carriers, including charge separation, migration, and interfacial transfer in photoelectric materials. Precise regulation of these dynamics is a crucial pathway for achieving high conversion efficiency. Addressing this key scientific challenge, we have developed novel spatiotemporally resolved detection methods to uncover the mechanisms in carrier dynamics. Furthermore, by employing external field regulation strategies (e.g., high pressure, low temperature), we have realized controlled rapid transport of photogenerated carriers within materials, significantly enhancing photodetection response. Building on this foundation, we constructed a dynamic research platform for optoelectronic devices, successfully applying these regulatory strategies to achieve highly efficient photoelectric conversion devices.

References

1. Xiao Y.*, Yan X., Cai R., Liu X, Bao J., Zhang M., Leng J.*, Jin S.*, Tian W.* Nat. Commun. 2025, 16, 8081.
2. Sun F., Deng Y., Leng J., Shi M., Li C., Jin S., Li R.*, Tian W.* J. Am. Chem. Soc. 2024, 146, 31106.
3. Yin Y., Yan X., Luo H., Liang Y., Xu P., Wang Y., Jin S., Tian W.* Angew. Chem. Int. Ed. 2024, e202418587.

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Ultrafast scattering & spectroscopy study on a photoinduced thermochemical reaction

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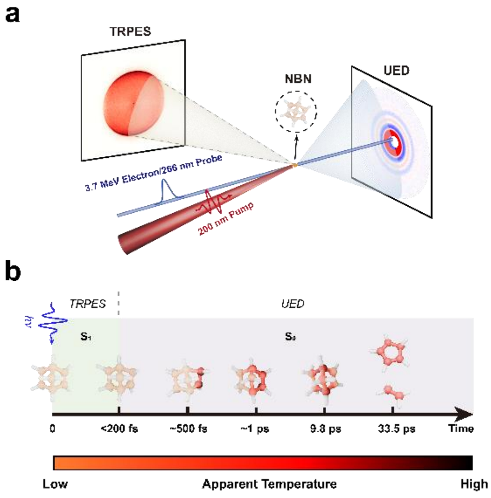
Keywords: Ultrafast electron diffraction, retro-Diels-Alder reaction

Abstract: While pump-probe methods have revolutionized the study of photoinduced dynamics, observing purely thermochemical reactions in real time remains a major challenge due to the difficulty of depositing energy on femtosecond timescales. In this talk, we demonstrate a new strategy to bridge this gap through a combined ultrafast electron diffraction and time-resolved photoelectron spectroscopy study of the norbornene retro-Diels-Alder (rDA) reaction. We find the reaction proceeds via a two-step mechanism: an initial photochemical step, featuring ultrafast internal conversion to a local C=C bond, is followed by a distinct 33-ps thermochemical rDA step on the opposite end of the molecule. These steps are separated by a 10-ps induction window where energy is redistributed via ring-puckering vibrations. The clean separation of reaction coordinates between photophysical internal conversion and thermochemical reaction provides a general framework for probing fundamental thermochemical processes on ultrafast timescales.



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Spin Manipulation and Coherence Transfer of Colloidal Nanoplatelets

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Keywords: Colloidal Nanoplatelets; Elemental Doping; Electronic Spin Relaxation; Inorganic/Organic Interface; Spin Coherence Transfer

Abstract: Quantum information technology refers to the technology that uses the quantum states of microscopic particles to represent information and utilizes quantum mechanical principles for information storage, transmission and processing. The electronic spin polarization of molecules is crucial for enhancing magnetic resonance signals and advancing molecular quantum information science. Among various low-dimensional semiconductor materials, two-dimensional colloidal nanoplatelets have emerged as ideal systems for optically injecting spin information due to their large heavy-light hole band splitting. Recently, we applied a copper ion elemental doping strategy to modulate the spin relaxation of nanoplatelets. By leveraging the rapid trapping of photogenerated holes by copper ions, we achieved room-temperature electronic spin coherence states with lifetimes of hundreds of picoseconds in the nanoplatelets, which can be further extended to several nanoseconds at low temperatures. Combined with naphthalimide electron acceptors, we realized efficient coherent transfer (~80%) of spin-polarized electrons from nanoplatelets to organic molecules. This study demonstrates a new approach to developing advanced quantum technologies by integrating semiconductor spin physics principles with molecular science, and provides important guidance for the construction of low-cost, near-room-temperature spin electronic and quantum information systems.

References

Wang, L., Wang, J.*, Sun, J., Lv, Y., Ding, T., Cheng, P., Wu, K.* *Nano Lett.,* 2025, 25, 5932.
Lin, X., Han, Y., Zhu, J., Wu, K.* *Nat. Nanotechnol.*, 2022, 18, 124.
Wang, L., Chen, Z., Liang, G., Li, Y., Lai, R., Ding, T., Wu, K.* *Nat. Commun.,* 2019, 10, 4532.

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Two-Dimensional Electronic Spectroscopy at 100 kHz Repetition Rate for Ultrafast Dynamics Study

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Keywords: Two-dimensional electronic spectroscopy, Energy transfer, Light-matter coupling.

Abstract: Ultrafast two-dimensional electronic spectroscopy is unique in investigating the coupling between different excited states of a system, charge and energy transfer processes as well as their dynamics with both high temporal and high frequency resolution. Using a high-speed camera, we achieve shot-to-shot detection at a high repetition rate (100 kHz), which significantly improves the acquisition efficiency and signal-to-noise ratio of the system. Based on this system, we investigated the coupling between surface plasmons of metals and excitons of organic semiconductor molecules. Plasmon-mediated exciton delocalization phenomenon under weak coupling conditions and coherent oscillation under strong coupling conditions were observed, which reflect the coherent energy transfer process between the matter and electromagnetic field mode. We have also conducted research on inorganic semiconductor materials, revealing a secondary Auger-assisted carrier transfer process in a type I $MoS_2/PtSe_2$ heterostructure. Specifically, when exciting the small bandgap $PtSe_2$, a distinct two-step rise is observed for the exciton signal of the large bandgap MoS_2. Recently, we have investigated the incoherent dynamics of exciton-polaritons in WSe_2 flake on an Au substrate and found that energy can be transferred back and forth between the exciton reservoir and lower polariton (LP) under different excitation conditions. That is, energy cascades from exciton state into LP when using high energy pumping and energy can transfer back from LP to exciton state when selectively exciting the LP. These results demonstrate the opportunity for novel functional optoelectronic and photocatalytic materials by manipulating light-matter coupling.

References

Timmer, D.; Gittinger, M. et al. *Nat. Commun.* 2023, 14 (1), 8035.
Niu Xu, Weiming Song, et al. *J. Mater. Chem. C,* 2024,12, 16332-16342

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Reaction and Structural Dynamics in the Blue-Light Photoreceptors

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Keywords: Proton-couple electron transfer, transient absorption, infrared

Abstract: The blue light using flavin (BLUF) domain is a widespread photoreceptor structural domain in microbial systems, which consists of a flavin cofactor that absorbs blue light, triggering a chemical reaction that can induce conformational changes in proteins like dominoes, and holds great promise as a tool for optogenetics. Currently, there are two important questions in the field of BLUF domains regarding its photoactivation mechanism. The first question is how to resolve the bidirectional proton-coupled electron transfer reaction containing six elementary steps on an ultrafast time scale, and the second question involves the structural changes of proteins triggered by the photochemical reaction, i.e. how the amino acids of the proteins undergo side-chain isomerization, hydrogen-bonding network reorganization, and side-chain displacement, among other motions to switch from the dark-state structure to a functional light-state structure. In the past several years, our group has mainly focused on the mechanism of proton-coupled electron transfer processes of the BLUF domain using transient UV-visible spectroscopy, and step-by-step resolved the temporal sequence, rates, kinetic isotope effects, and coupling of the six elementary steps within the reaction by mutant design. The fundamental understanding of the reaction dynamics, in turn, has facilitated a cross-species mechanism of the BLUF domain, which has been a central problem in this field. Our work shows that despite the diverse kinetic results acquired for different species of BLUF domain, their mechanisms can be rationalized within a unified framework, wherein the diversity results from the sensitivity of proton transfer reaction rates to the distances of hydrogen bonds within the active site. Currently, our group has been working on the development of mid-infrared (MIR) spectroscopy-based techniques, *i.e.*, transient mid-infrared (TRIR) spectroscopy and two-dimensional infrared (2DIR) spectroscopy, to further monitor the structural dynamics in the BLUF domain, such as probing the hydrogen bonding rearrangement within the active site with the incorporation of site-specific infrared probes.

References

Kang, X.-W., Wang, K., Zhang, X., Zhong, D.*, Ding, B.*, Elementary Reactions in the Functional Triads of the Blue-Light Photoreceptor BLUF Domain. *J. Phys. Chem. B* **2024**, 128, 2065

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Nonlinear optical spectroscopy of oxide/water interfaces

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Keywords: oxide/water interface; sum-frequency vibrational spectroscopy

Abstract: The interface between oxides and liquid water is ubiquitous on Earth, shaping our landscape and playing a crucial role in the global carbon cycle. Moreover, in various current renewable energy solutions, the oxide-water interface also assumes significant roles, such as serving as electrocatalysts for hydrogen and oxygen evolution reactions. In recent years, thanks to the theoretical and experimental advances, people have gained remarkable progress in the fundamental understanding on such solid-liquid interfaces. By developing new nonlinear spectroscopy experimental methods, we have enabled in situ detection of the evolution and reconstruction of oxide surface lattices inside liquid water under ambient conditions, uncovering unique interface structures and reaction pathways that differ from conventional ones [1]. On this basis, we have gained new insights into the electrical properties, hydration reactions, isotope effects, and interactions with solution ions at oxide-water interfaces, which will inform our discussions on related applications.

References

X. Li *et al*., *Unconventional structural evolution of an oxide surface in water unveiled by in situ sum-frequency spectroscopy,* Nature Chemistry **17**, 198~203 (2025).

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Open system quantum dynamics and spectroscopy in molecular systems with strong light-matter coupling

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Keywords: Hierarchical equations of motion, Molecular polariton, Plexciton

We present our recent theoretical work on strongly coupled light-matter systems in both microcavity and plasmonic systems, focusing on the dynamics and spectroscopy of polaritons and plexcitons. In the first part, we construct a path integral framework for the Dicke and Tavis–Cummings models in the thermodynamic limit, in which the collective molecular response is mapped onto an effective harmonic bath. This description provides a unified way to include static disorder and vibronic coupling, and enables efficient simulations of absorption spectra and polariton dynamics using hierarchical equations of motion (HEOM) and exact diagonalization. Because the effective harmonic bath model cannot describe nonlinear optical responses, we additionally employ a quantum master equation to calculate pump-probe spectra and track the bright-state dynamics of molecular polaritons. In the second part, we extend the HEOM approach to plexciton systems, where a two-level exciton interacts with a short lived plasmonic mode. Our calculations show that, as the coupling strength increases, the absorption profile evolves from an asymmetric Fano shape to a Rabi-split doublet, while vibronic coupling tends to symmetrize the spectrum. Simulated two-dimensional electronic spectra further reveal nonlinear signatures specific to plexcitons, including a characteristic breathing-mode pattern that serves as a spectroscopic marker of Rabi oscillations.

References:

[1] T.-C Li, C.-H. Huang, S.-M. Bai, Q. Shi, J. Chem. Phys. 162, 094105 (2025).

[2] C.-H. Huang, S.-M. Bai, Q. Shi, J. Chem. Theory Comput. 21, 3612 (2025).

[3] Y.-L. Ding, C.-H. Huang, Y.-J. Chen, S.-M. Bai, Q. Shi, submitted.

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Out of the Blue: Discovery and Application of a Blue Fluorescent Amino Acid

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Keywords: Fluorescence spectroscopy and microscopy, unnatural amino acid, tryptophan

Abstract: Fluorescence-based spectroscopic and imaging techniques play an essential role in biological research. However, since most biological molecules lack a suitable fluorescent group, fluorescent labelling is often required. To meet diverse needs and applications, researchers have developed a wide range of fluorescent tags, such as fluorescent dyes and fluorescent proteins. Although some of these fluorescent tags have been widely used in biological science, they have limitations when used to study proteins. This is because they either cannot be placed in the interior of proteins or can cause significant perturbation towards the native structure and/or function of the protein system in question. To overcome this limitation, researchers have attempted to develop fluorescent reporters based on simple modification of natural amino acids (e.g., tryptophan). In this talk, we will discuss some of our work in this area, primarily focusing on the development of a tryptophan-based blue fluorescent unnatural amino acid, including its photophysical property, protein incorporation, and applications in biological spectroscopy and microscopy.

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Femtosecond Broadband Transient Fluorescence Spectroscopy

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Keywords: Femtosecond transient fluorescence; Parametric superfluorescence; Vibronic coupling; Chlorophyll excited states; Photosynthetic protein systems

Abstract: The femtosecond time-resolved transient fluorescence spectrometer, based on the principle of non-collinear optical parametric amplification (NOPA), possesses unique advantages including high temporal resolution, high gain, broad measurement bandwidth, and low detection limit. However, parametric superfluorescence (PSF), originated from the intensity fluctuations of vacuum quantum noise introduced during the optical parametric amplification process, constitute the primary noise source, significantly limiting the instrument's ability to detect weak transient fluorescence signals. We propose and implement for the first time a femtosecond fluorescence conical optical parametric amplification spectroscopy (FCOPAS), which enables effective cancellation of noise fluctuation across the entire PSF ring, resulting in an approximate order of magnitude reduction in PSF noise compared to prior NOPA outcomes. This breakthrough enables the detection of previously undetectable weak transient signals. Utilizing this advanced technique, we have experimentally observed the transient fluorescence dynamics of chlorophyll molecular excited states and various photosynthetic protein systems. These observations have revealed key ultrafast dynamical processes within these systems, including energy transfer, charge separation, and vibrational cooling.

References

Cui, E., Liu, H., Wang, Z., Chen, H., Weng, Y., *Rev. Sci. Instrum.* 2024, 95, 033008.
Liu, H., Ruan, M., Mao, P., Wang, Z., Chen, H., Weng, Y., *J. Chem. Phys.* 2024, 160, 205101.

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Time-resolved dynamics of metal halide perovskite under high pressure

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Keywords: self-trapped exciton, electron-phonon coupling, the diamond anvil cell

Metal halide perovskites have garnered significant attention in the scientific community for their promising applications in optoelectronic devices. The application of pressure engineering, a viable technique, has played a crucial role in substantially improving the optoelectronic characteristics of perovskites. Despite notable progress in understanding ground-state structural changes under high pressure, a comprehensive exploration of excited state dynamics influencing luminescence remains incomplete. This report introduces recent advances in time-resolved dynamics studies of photoexcited metal halide perovskites under high pressure. With a focus on the intricate interplay between structural alterations and electronic properties, we investigate electron−phonon interactions, carrier transport mechanisms, and the influential roles of self-trapped excitons (STEs) and coherent phonons in luminescence. However, significant challenges persist, notably the need for more advanced measurement techniques and a deeper understanding of the phenomena induced by high pressure in perovskites.

References

1. Jiang, J. T.; Niu, G. M.; et al.; Yuan, K. J.*; Yang, X. M. Adv Func Mater **2023,** 2312316.

2. Niu, G.; Jiang, J.; et al.; Yuan, K. J.*; Yang, X. M. J Phys Chem Lett **2024,** 15, 1623-1635.

3. Niu, G.; Jiang, J.; et al.; Yuan, K. J.*; Yang, X. M. Angew Chem Int Ed **2025,** e202422424.

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Post-OPA Enhanced SFG Spectroscopy and Transient Absorption Microscopy

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Here, I present an innovative enhancement technique of sum frequency generation (SFG) vibrational spectroscopy, using a picosecond noncollinear optical parametric amplifier (NOPA).[1] We conducted a systematical investigation into the impact of different intensities of pump and SFG seed light, as the input signal in NOPA, and demonstrated this method on the octadecanethiol (ODT) molecules on gold films. The amplified SFG by NOPA reproduced the SFG vibrational spectra, enhanced by about 4 orders of magnitude but with broader spectral resolution due to the short pulse width of the pump light in NOPA. Recently, we are developing highly sensitive transient absorption microscopy (TAM) and SFG spectroscopy. I will introduce some of our recent progresses.

1. Zeng, W.; Li, B.-H.; Zeng, W.-W.; Zhou, C.; Yang, X.; Ren, Z., Noncollinear Optical Parametric Amplification of Broadband Infrared Sum Frequency Generation Vibrational Spectroscopy. *J. Phys. Chem. Lett.* **2024,** *15*, 2470-2475.

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A Multi-Agent System for Complex Chemical Reaction Information Extraction

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The extraction of structured chemical information from literature is essential for constructing reaction databases that drive data-driven and AI-powered chemical research. A major challenge lies in the multimodal and complex nature of chemical data. In order to convert the raw data into structured, machine readable datasets, a modeling framework is needed with the ability to comprehend text, tables, and graphical representations of molecular structures. Existing approaches predominantly focus on single tasks [1-3], limiting their ability to fully capture reaction details and leading to incomplete datasets.

To overcome this, we present ChemEagle, a multimodal large language model (MLLM)-based multi-agent system that integrates diverse chemical information extraction tools. By integrating seven expert-designed tools and six chemical information extraction agents, ChemEagle not only processes individual modalities but also utilizes MLLMs' reasoning capabilities to unify extracted data, ensuring more accurate and comprehensive reaction representations. We demonstrated the model's capability in parsing chemical reaction diagrams, converting molecular structures to SMILES, and substituting functional groups or molecular fragments from tabulated lists. In all these tasks our model performed better than existing methods by a significant margin. Our approach presents a significant step towards automated chemical knowledge extraction, facilitating more robust AI-driven chemical research.

Reference

[1] Guo, J.; Ibanez-Lopez, A. S.; Gao, H.; Quach, V.; Coley, C. W.; Jensen, K. F.; Barzilay, R. Automated chemical reaction extraction from scientific literature. *J. Chem. Inf. Model.* **62**, 2035-2045 (2021).
[2] Vaucher, A. C.; Zipoli, F.; Geluykens, J.; Nair, V. H.; Schwaller, P.; Laino, T. Automated extraction of chemical synthesis actions from experimental procedures. *Nat. Commun.* **11**, 3601 (2020).

[3] Qian, Y.; Guo, J.; Tu, Z.; Coley, C. W.; Barzilay, R. RxnScribe: A sequence generation model for reaction diagram parsing. *J. Chem. Inf. Model.* **63**, 4030-4041 (2023).

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Multi-State Density Functional Theory for Ground and Excited States

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Keywords: Density Functional Theory; Excited States; Strong Correlation

With good balance between computational accuracy and efficiency, density functional theory (DFT) has been an indispensable tool for scientists in chemistry, physics and materials. However, DFT has been insufficient in describing general excited states and systems with strong electronic correlation. Therefore, it is a demanding challenge in theoretical chemistry to develop a universal approach based on DFT for simulation of excited states. We report a rigorous formulation of multi-state density functional theory (MSDFT) that treats ground and excited states on an equal footing. We establish the fundamental theorems of MSDFT. First, we prove the existence of a Hamiltonian matrix functional $\mathcal{H}[D]$ of the multi-state matrix density D(r) in the N-dimensional Hilbert subspace V^N. Then, we establish the variational principle of MSDFT, which states that variational minimization of the subspace energy, equal to the trace of $\mathcal{H}[D]$, with respect to the matrix density D(r) yields both the exact eigen-energies and densities of the N lowest eigenstates. Next, we show that the Hamiltonian matrix functional $\mathcal{H}[D]$ can be explicitly constructed by introducing a minimal active space (MAS), accompanied by the correlation matrix functional $\mathcal{E}^c[D]$, which accounts for correlation effects outside the MAS [2-3]. Approximated methods based on the framework of MSDFT have been successfully applied to simulate excited-state properties of systems with weak and strong correlation. These findings reveal the intricate structure of electronic correlation within the Hilbert subspace of lowest eigenstates and suggest a promising direction for efficient simulation of excited states.

References:

1. **Lu, Y.*** & Gao, J.* Multi-state density functional theory of excited states, *J. Phys. Chem. Lett.* **13**, 33, 7762 (2022).
2. **Lu, Y.*** & Gao, J.* Multistate Density Functional Theory: Theory, Methods, and Applications, *WIREs: Comput. Mol. Sci.* **15**, e70043 (2025).

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Reaction Mechanisms on Selected Photocages

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Keywords: Time-Resolved Spectroscopy; DFT Calculations; Photochemical Reaction Mechanism; Ultrafast Dynamics

Abstract: The mechanistic study of photochemical reactions of organic molecules lies at the intersection of organic physical chemistry and chemical kinetics. Because reactive intermediates may be toxic and can trigger side reactions, elucidating reaction mechanisms has significant practical value. Moreover, mechanistic insights are essential for regulating reaction efficiency and guiding molecular design. However, mechanistic investigations of photochemical processes remain challenging due to the complexity of excited-state pathways and the low concentration and short lifetimes of reactive intermediates. To address these challenges, the key is to obtain the molecular structures of the crucial intermediates. Our research group has developed an approach to studying photochemical mechanisms in organic molecules by combining time-resolved absorption spectroscopy and time-resolved resonance Raman spectroscopy with theoretical calculations. In this conference, I will present our recent mechanistic investigations on photocages. These mechanistic studies provide important insights for the improvement and development of multifunctional molecular designs and will further promote the application of these photochemical processes in biochemical contexts.

References

1. Y. Su, D. Zheng, L. Ge, L. Yu,* D. L. Phillips, J. Ma, * Y. Fang. *Chem. Sci.*, **2024**, *15*, 20556..
2. Y. Su, X. Li, D. Zheng, J. Andreásson, H. Wang, L. Yu,* J. Chen,* J. Ma,* and Y. Fang. *Chem. Sci.*, **2025**, DOI: 10.1039/d5sc06627a
3. Y. Cheng, S.-L. Zhang, J. Lammert, L. Yu, Y. Zhao, A. Studer *, J. Ma *, and Y. Fang. *JACS Au*, **2025**, DOI: 10.1021/jacsau.5c01342.

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Mechanism of aggregation-induced emission and control of excited state dynamics

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Abstract: The aggregation of molecules into nanostructures often results in fluorescence quenching, whereas a small group of exceptions do the opposite. Using ultrafast uv-vis and infrared multi-pulse mixing sequences and non-linear spectroscopic techniques, we carried out a detailed study of the evolution dynamics of molecular electronic excited states, revealing the mechanism of aggregation-induced emission of TPE molecules, and discovering that the fluorescence of the AIE molecules are of anti-Vavilov's rule. Based on the mechanism, we are able to tune photochemical reactions by mode-selective vibrational excitations.

References

[1] J Guan, X Li, C Shen, Z Zi, Z Hou, C Hao, Q Yu, H Jiang, Y Ma, Z Yu, J Zheng. (2024) Vibrational-Mode-Selective Modulation of Electronic Excitation, ChemPhysChem, e202400335.

[2] Q Yu, X Li, C Shen, Z Yu, J Guan, J Zheng. (2024) Blue-Shifted and Broadened Fluorescence Enhancement by Visible and Mode-Selective Infrared Double Excitations, J. Phys. Chem. A 128, 2912-2922.

[3] J Peng, X He, Y Li, J Guan, B Wu, X Li, Z Yu, J Liu, J Zheng. (2023) Restriction of Crossing Conical Intersections: The Intrinsic Mechanism of Aggregation-Induced Emission. Phys. Chem. Chem. Phys. 25, 12342-12351.

[4] Zhuowei Hou, Jianxin Guan, Jie Peng, Xinmao Li, Zhihao Yu, and Junrong Zheng. (2022) Double crossing conical intersections and anti-Vavilov fluorescence in tetraphenyl ethylene. The Journal of Chemical Physics, 156, 144302.

[5] J Guan, C Shen, J Peng, J Zheng. (2021) What Leads to Aggregation-Induced Emission? J Phys Chem Lett. 12, 4218.

[6] Guan, J.X., Prlj, A., Wei, R., Peng, J., Lin, K.H., Liu, J.T., Han, H., Yu, Z.H., Corminboeuf, C., Zhao D., and Zheng, J.R. (2020) Direct observation of aggregation-induced emission mechanism, Angew. Chem. Int. Ed., 59, 14903.

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Ultrafast charge carrier dynamics in metal halide perovskites by Terahertz spectroscopy

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Keywords: Terahertz spectroscopy, charge transport, ultrafast dynamics, charge transfer

Abstract: Solution-processed metal halide perovskites (MHPs) have gained tremendous research interest in recent years due to their outstanding photovoltaic performance, with a certified single-junction power conversion efficiency over 26%. Despite being low-temperature solution-processed, lead halide perovskites show exceptional optoelectronic properties, such as long carrier lifetime, remarkable defect tolerance *et.al*. Using time-domain terahertz spectroscopy, we have unveiled key optoelectronic characteristics of MHPs and their heterostructures including strong electron-phonon interactions, superior hot carrier transport and ultrafast optically controlled charge transfer.[1-3] These findings provide fundamental insights into the photophysical processes in MHPs, and may guide the development of next-generation perovskite-based optoelectronic applications.

References

1. **Zhang, H.**, Debroye, E., Zheng, W., Fu, S., Virgilio, L. D., Kumar, P., Bonn, M. & Wang, H. I. *Science Advances*, 2021, 7, eabj9066.
2. **Zhang, H.**, Debroye, E., Fu, S., González, M. C. R., Feyter, S. D., Hofkens, J., Bonn, M., & Wang, H. I. *Advanced Materials*, 2023, 2211198.
3. Chen, Q.[#], Lodi, A.[#], **Zhang, H.**[#], Gee, A., Wang, H. I., Kong, F., Clarke, M., Edmondson, M., Hart, J., O'Shea, J. N., Stawski, W., Baugh, J., Narita, A., Saywell, A., Bonn, M., Mullen, K., Bogani, L. & Anderson, H. L. *Nature Chemistry*, 2024, 16, 1133-1140.

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Multi-Modal Ultrafast Nonlinear (Vibrational) Spectroscopy for AI Future

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Keywords: Nonlinear spectroscopy; Multi-modal; Vibrational spectroscopy; Artificial intelligence.

Abstract: We present a multi-modal ultrafast nonlinear spectroscopy platform that synergistically combines high-resolution techniques including sum-frequency generation, IR, and coherent Raman spectroscopies. By synchronizing picosecond and femtosecond lasers, we achieve sub-wavenumber resolution with high accuracy and exceptional signal-to-noise ratio (SNR) across all modalities. This performance generates a rich stream of high-fidelity, multi-dimensional vibrational data -a "big data" source ideally suited for artificial intelligence (AI). This convergence may provide a powerful paradigm for AI-driven discovery, enabling the decoding of complex molecular structures and ultrafast dynamics at interfaces and in condensed phases with unprecedented insight.

References

1. Li Zhang, Luo-Zhou Chen, Bo-Jun Zhao, Ze-Kun Zhang, Jing-Ming Cao, Hui Wang, Xiao-Hua Hu, Zheng-Tang Liu, Xing-Xing Peng, An-An Liu, and Hongfei Wang*. Sub-1 cm-1 high-resolution broadband sum-frequency generation vibrational spectroscopy (HR-BB-SFG-VS) with significantly improved sensitivity and signal-to-noise ratio (SNR). J. Chem. Phys. 163, 104201 (2025)
2. Li Zhang, Bo-Jun Zhao, Jin-hua Jiang and Hongfei Wang*. Quantitative consistency between the intensity and phase-resolved sum frequency generation vibrational spectra of the air/neat-water interface. J. Chem. Phys. 163, 034703 (2025).
3. Hong-fei Wang*, Luis Velarde, Wei Gan, Li Fu, Quantitative Sum-Frequency Generation Vibrational Spectroscopy of Molecular Surfaces and Interfaces: Lineshape, Polarization, and Orientation, Annu. Rev. Phys. Chem., 66, 189-216, 2015.

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Anion Recognition Investigated by Linear and Nonlinear Vibrational Spectroscopy

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Keywords: Anion Recognition, Structural Dynamics, Ultrafast IR Spectroscopy

Abstract: In this talk, the ultrafast structural dynamics and nonlinear spectroscopic study of ion recognition in solution will be presented. By constructing host-guest interaction systems and studying the dynamics between anions and macrocyclic receptors using linear and nonlinear vibrational spectroscopy techniques, it was found that enthalpy change is the main driving force for anion recognition. Additionally, the reorientational time constant of anions and the activation energy of rotational relaxation dynamics processes during the ion recognition were first reported. Through the combination of theoretical analysis and experimental results, it was revealed that reorientational dynamics is controlled by solvent viscosity and the anion recognition achieved through rearrangement of hydrogen bond structures. This study, based on the framework of classical thermodynamics and ultrafast dynamics, provides insightful guidance for future supramolecular chemistry research and is of great significance for better understanding ion transport and regulation in life processes.

References

[1] Zhang, F.; Bian, L.; Peng, J.; Li, J.; Qu, Y.; Bian, H. T.* ***J. Phys. Chem. Lett.*** 2025, 16: 11752-11761.
[2] Zhou, D.; Zhang, F.; Wang, B. H.; He, J. M.; Bai, Y.; Bian, H. T.* ***J. Phys. Chem. Lett.*** 2023, 14: 11183-11189.
[3] Zhou, D.; Zhao B.; Bai, Y.; Mukherjee, S.; Liu, J.*; Bian, H. T.*; Fang, Y. ***J. Phys. Chem. Lett.*** 2022, 13: 669-675.

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Ultrafast Vibrational Signatures of Conformationally Gated Phase Separation in a Natural Folded Enzyme

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Keywords: two-dimensional infrared (2D-IR); stimulated Raman scattering (SRS); molecular dynamics; Liquid–liquid phase separation (LLPS);

Abstract:

Liquid–liquid phase separation (LLPS) underpins the formation of biomolecular condensates that organize cellular biochemistry. While most known examples arise from intrinsically disordered proteins (IDPs), we show that the folded metabolic enzyme Lipoate-protein ligase A (LplA) undergoes reversible, conformation-gated LLPS.[1] Only the catalytically inactive bent state phase-separates, whereas the extended active state remains dispersed—revealing a direct mechanistic link between conformational energetics and condensate formation. To capture the multiscale dynamics underlying this behavior, we combine ultrafast two-dimensional infrared (2D-IR) spectroscopy[2], stimulated Raman scattering (SRS) imaging, and multiscale molecular dynamics simulations. 2D-IR measurements show a continuous LCST-type transition with gradually evolving amide-I, indicating progressive conformational rearrangement rather than cooperative unfolding. SRS imaging provides label-free, chemically selective mapping of the emerging condensates, revealing spatial heterogeneity in α-helical density and hydration. Simulations reveal that the bent and extended states expose the enzyme's intrinsically disordered region (IDR) in distinct orientations, altering interaction valency and interfacial water structure. Point mutations that perturb these IDR orientations modulate both hydration dynamics and macroscopic LLPS behavior, validating a conformation–IDR–solvent coupling mechanism. Overall, our results demonstrate that reversible conformational transitions in folded enzymes can act as molecular gatekeepers for LLPS, and that ultrafast vibrational spectroscopy provides a direct route to linking sub-picosecond hydrogen-bond dynamics to mesoscale condensate formation.

References

1. Nie, J.; Zhang, X.; Hu, Z.; Wang, W.; Schroer, M. A.; Ren, J.; Svergun, D.; Chen, A.; Yang, P.; Zeng, A. P. *Nat Commun* **2025,** 16, (1), 2449.
2. You, X.; Shirley, J. C.; Lee, E.; Baiz, C. R. *Cell Rep Phys Sci* **2021,** 2, (5).

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Algorithm-Driven Robotic Discovery of Polyoxometalate-Based Metal-Organic Frameworks

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Keywords: algorithm-driven discovery, robotic synthesis, metal-organic frameworks

Abstract: The experimental exploration of chemical space of crystalline materials requires a large set of reactions and the multiparameter control. Especially, the synthesis of metal-organic frameworks (MOFs) involves complex and labor-intensive processes. To address these challenges, we developed a modular robotic system integrated with customized machine-learning models, including an XGBoost-based feedback loop and multi-class classification, to efficiently explore the polyoxometalate-based MOFs (POMOFs) chemical space.[1] This closed-loop strategy focuses on high-uncertainty regions, generates detailed chemical-space maps, and guides targeted synthesis. All robotic operations are encoded in the universal χDL language,[2] ensuring reproducible crystallization and yields. By combining automated synthesis, algorithmic decision-making, and data-rich outputs, this platform could enable scalable POMOF discovery and provide compositionally controlled samples with well-defined structures, ideal for future AI-enhanced ultrafast spectroscopy and next-generation structure–dynamics–function studies.

References

1. He, D.; Jiang, Y.; Guillen-Soler, M.; Geary, Z.; Vizcaino-Anaya, L.; Salley, D.; Gimenez-Lopez, M. D. C.; Long, D.-L.; Cronin, L. *J. Am. Chem. Soc.* 2024, 146, 28952-28960.
2. Mehr, S. H. M.; Craven, M.; Leonov, A. I.; Keenan, G.; Cronin, L., *Science* 2020, 370, 101-108.

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Exciton Delocalization and Transport in Layered Semiconductors

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Keywords: 2D semiconductor, ultrafast imaging, hot carrier, delocalization

Abstract: Two-dimensional (2D) layered semiconductors exhibit unique optical responses and electronic structures at the atomic scale. Directly probing carrier transport in these materials is critical for understanding their energy conversion mechanisms and guiding the development of high-performance optoelectronic devices. Here, we employ ultrafast imaging to visualize charge carrier dynamics in both transition metal dichalcogenides (TMDCs) and 2D halide perovskites. We observe rapid picosecond hot-carrier diffusion in WS_2 and WSe_2, in contrast to MoS_2 and $MoSe_2$, where such behavior is largely absent. The transport characteristics further depend strongly on thickness and interfacial environment. In 2D perovskites, subtle changes in lattice rigidity significantly modify the exciton energy landscape, leading to different dominant transport pathways, from thermally activated hopping in $(BA)_2PbI_4$ to band-like motion in $(PEA)_2SnI_4$. These results provide insights into charge and exciton behavior in layered semiconductors and support future device optimization.

References

[1] Wei et al. Lattice Control of Exciton Landscapes Enhances Carrier Transport in 2D Perovskites, submitted, 2025.
[2] Yuan et al. Strong Dipolar Repulsion of One-Dimensional Interfacial Excitons in Monolayer Lateral Heterojunctions, *ACS Nano* 17, 16, 15379–15387 (2023)
[3] Yuan et al. Twist-angle-dependent interlayer exciton diffusion in WS_2–WSe_2 heterobilayers. *Nature Materials* 19, 617–623 (2020)

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Title Construction of Chemical Reaction Networks Driven by Both AI and Physics

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Keywords: Chemical reaction network; Machine learning; Reaction pathway

Abstract: The origin of life on Earth remains a major scientific mystery. While many bottom-up experiments under prebiotic conditions have provided insights into life's spontaneous chemical origin, understanding of complex reaction processes remains limited. Herein, we propose a novel approach using a Rotation-Translation Invariant Potential (RTIP) formalized purely in Cartesian coordinates to enable automated chemical reaction simulation. Employing RTIP path sampling to explore primitive molecule reactivity, we identified several low-energy reaction mechanisms, including dihydrogen transfer hydrogenation and HCOOH-catalyzed hydration/amination. These efforts constructed a comprehensive reaction network illustrating synthetic pathways of glycine, serine, and alanine. Further thermodynamic analysis highlights methylenimine as a crucial precursor for amino acid synthesis, as it exhibits more favorable reactivity in coupling reactions than the traditionally recognized hydrogen cyanide. Our study demonstrates that the RTIP method combined with a divide-and-conquer strategy provides a new perspective for simulating complex reactions and a valuable tool for advancing research on reaction mechanisms in complex systems.

References

1) Li, B.; Xiao, J.; Gao, Y.; Zhang, J. Z. H.; Zhu, T.* J. Chem. Inf. Model. 2025, 65, 2297.

2) Xiao, J.; Zhang, Y.; Li, B.; Zhang, S.; Gao, Y.; Chen, W.; Wang, H.; Zhang, J. Z.*; Zhu, T.* JACS Au 2025, 5, 3892.

3) Zhang, Y.*; Xiao, J.; Wang, S.; Zhu, T.*; Zhang, J. Z.* J. Chem. Theory Comput. 2025, 21, 3410.

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Excited State Dynamics of Metal Nanoclusters

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Keywords: nanoclusters, ultrafast spectroscopy, dynamics

Abstract: Atomically precise metal nanoclusters consist of tens to hundreds of metal atoms, which bridge the metallic and non-metallic nanoparticles. In this talk, I will introduce our recent work on the ultrafast dynamics of metal nanoclusters including: (1) The evolution from discrete energy levels to continuous band in metal nanoclusters. (2) Triplet state energy transfer and utilization in metal nanoclusters. (3) Coherent vibrational dynamics of metal nanoclusters. Our results indicates that metal nanoclusters provide a good platform for understanding the evolution of excited properties of nanomaterials.

References

1. Shi, W.-Q.; Zeng, L.; He, R.-L.; Han, X.-S.; Guan, Z.-J.; Zhou, M.*; Wang, Q.-M.*, Science 2024, 383, 326-330.

2. Zhang, W.; Luo, L.; Liu, Z.; Zhao, F.; Kong, J.*; Jin, R.*; Luo, Y.; Zhou, M.*, Sci. Adv. 2025, 11, eadx2781.

3. Zhang, W.*; Kong, J.; Liu, W.-T.; Zhao, R.; Zhang, J.; Deng, H.; Lei, Z.*; Wang, Q.-M.; Luo, Y.; Zhou, M.*, Angew. Chem. Int. Ed. 2025, 64, e202515551.

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What is the redox state of a dual function CraCRY?

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Keywords: photoenzyme dynamics, structural signaling, DNA repair, single-molecule kinetics

Abstract: The recent discovered bifunctional cryptochromes are significant with drastic dual functions for signal transduction as a photoreceptor and for DNA repair as a photoenzyme. We have recently characterized DNA repair with femtosecond spectroscopy and revealed the repair photocycle with determining all critical timescales. As observed in other photolyases, the redox state for repair function is a fully reduced hydroquinone ($FADH^-$) but for photoreceptor, it usually is the oxidized state FAD. For a dual function CraCRY, what is the functional redox state in cell? Using single-molecule electric detection, we studied the C-terminal structural fluctuation for signaling and DNA recognition for repair at different redox states. We aim to rationalize a common redox state for both functions in cell.

References

1. L. Yan, X. Cao, L. Wang, J. Chen, A. Sancar and D. Zhong, *PNAS* (2024) 121, e2417633121. Dynamics and mechanism of DNA repair by a bifunctional cryptochrome.

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Regulation and Application of Exciton Kinetics in Colloidal Quantum Dots

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Keywords: quantum dots, hybrid materials, energy transfer, exciton kinetics regulation.

Abstract: Quantum dots (QDs) have emerged as highly promising luminescent materials due to their large extinction coefficients and precisely tunable absorption and emission wavelengths. However, conventional QD systems still face several critical challenges, such as short exciton lifetimes and pronounced reabsorption effects, which significantly limit their practical performance.

In this study, we demonstrate a precise regulation of exciton kinetics in QDs by constructing QD–molecule hybrid systems. Specifically, we realized rapid energy transfer from QD excitonic states to the molecular triplet states, enabling temporary storage of excitonic energy in long-lived molecular triplets. The stored triplet energy can then be re-injected into the QD exciton states through an endothermic reverse energy transfer process. Benefiting from this cyclic energy management mechanism, the QD exciton lifetimes were remarkably prolonged by four orders of magnitude, reaching the ~100 μs timescale. Furthermore, by tailoring different QD–molecule hybrid systems, we successfully achieved the prolonged exciton lifetime across a broad spectral range from the ultraviolet to NIR region. Such prolonged excited-state lifetimes substantially enhance the efficiency of photocatalytic processes.

To address the intrinsic reabsorption effect commonly observed in QD systems, we further developed QD–AIEgen hybrid systems. Through efficient energy transfer from QDs exciton to the AIEgen singlet, the Stokes shift of the luminescent material was significantly expanded from approximately 10 nm to ~120 nm, effectively eliminating reabsorption. In addition, the hybrid material exhibited excellent photostability and a near-unity PLQY. Owing to these outstanding properties, this luminescent system demonstrated superior performance and great potential in luminescent solar concentrators.

References

(1) **He, S.**; Wu, K.* *Angew. Chem., Int. Ed.* **2025**, e202423960.
(2) Liang, G.*; **He, S.** *; Wu, K.* *J. Am. Chem. Soc.* **2025**, *147*, 7974-7982.
(3) **He, S.**; Tang B. Z.*; Wu, K.* *Angew. Chem., Int. Ed.* **2025**, e202506555.

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Time-dependent absorption and emission spectra in organic charge- and energy-transfer systems

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Keywords: time-resolved spectroscopy, exciplex dynamics, charge transfer

Abstract: The distinction between ground-state charge-transfer complexes (CTCs) and excited-state complexes (exciplexes) is often blurred in organic donor-acceptor systems. Here employ time-dependent emission and absorption spectroscopies to visualizethe dynamic evolution of these transient species in naphthalimide-amine systems. We report the discovery of a "photo-induced charge-transfer complex" (PCTC), a kinetically trapped ground-state species formed between an amine and an imide. Using time-resolved photoluminescence mapping, we track the transition from an initial encounter exciplex to a stable, solution-persistent PCTC. We then extend this approach to the fluorochromic sensing of tertiary amines and opioids. By analyzing the temporal evolution of emission spectra, we differentiate between dual-emissive pathways: those arising from static ground-state pre-association and those resulting from diffusion-controlled excited-state interactions.

References

1. Huang, W.; Zhang, X.; Su, H.; Zhang, B.; Feng, A.; Jiang, J.; Chen, B.; Zhang, G. Trapping Highly Reactive Photo-Induced Charge-Transfer Complex Between Amine and Imide by Light. *Chem* **2024**, *10*, 2683–2696.
2. Chen, X.; Zhu, R.; Zhang, B.; Zhang, X.; Cheng, A.; Liu, H.; Gao, R.; Zhang, X.; Chen, B.; Ye, S.; Jiang, J.; Zhang, G. Rapid room-temperature phosphorescence chiral recognition of natural amino acids. *Nat. Commun.* **2024**, *15*, 3314.
3. Cheng, A.; Gu, X.; Yang, C.; Liu, M.; Zhang, B.; Liu, H.; Chen, X.; Feng, A.; Smith, P. E. S.; Jiang, J.; Luo, Y.; Huang, W.; Zhang, G. Rapid Fluorochromic Sensing of Tertiary Amines and Opioids via Dual-Emissive Ground and Excited Charge-Transfer States. *J. Am. Chem. Soc.* **2025**, *147*, 13512–13521.

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Nonadiabatic Dynamics of Ultrafast Intersite Charge Transfer during Chemical Bond Formation: Hydrogen Scattering from a Semiconductor Surface

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Keywords: Ultrafast Charge Transfer; Nonadiabatic Dynamics; Semiconductor Surface

Abstract: A first-principles coupled electron-nuclear dynamics simulation based on real-time, time-dependent density functional theory and Ehrenfest dynamics quantitatively reproduces bimodal translational energy loss and angular distributions observed in experiment for hydrogen atom scattering from Ge(111)-*c*(2×8). The theory elucidates a site-selective mechanism of electronically nonadiabatic energy transfer associated with the formation of different Ge-H bonds. This nuclear-to-electronic energy transfer observed in this system reflects the electronic dynamics of covalent bond formation at a semiconductor surface, a mechanism that is quite distinct from previously identified nonadiabatic energy transfer mechanisms at metal surfaces mediated by electronic friction or transient negative ions.

References

1. Krüger, K.; Wang, Y.; Tödter, S.; Debbeler, F.; Matveenko, A.; Hertl, N.; Zhou, X.; **Jiang, B.**; Guo, H.; Wodtke, A. M.; Bünermann, O., Hydrogen atom collisions with a semiconductor efficiently promote electrons to the conduction band. *Nat. Chem.* **2023,** *15* (3), 326-331.

2. Krüger, K.; Wang, Y.; Zhu, L.; **Jiang, B.**; Guo, H.; Wodtke, A. M.; Bünermann, O., Isotope effect suggests site-specific nonadiabaticity on Ge(111)c(2×8). *Nat. Sci.* **2024,** *4* (1), e20230019.

3. Zhu, L.; Zheng, Q.; Wang, Y.; Krüger, K.; Wodtke, A. M.; Bünermann, O.; Zhao, J.; Guo, H.; Jiang, B., Mechanistic Insights into Nonadiabatic Interband Transitions on a Semiconductor Surface Induced by Hydrogen Atom Collisions, *JACS Au* **2024,** *4*, 4518-4526.

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Femtosecond optics and X-ray lasers and its application in ultrafast dynamics research

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Keywords: Femtosecond optics, XFEL

Advanced experimental methods with high spatial-temporal resolutions are essential for ultrafast dynamics at microscopic scales, primarily focusing on the movements of individual electrons or nuclei. The rapid development of Xray free-electron lasers (XFELs) has created a new foundation for ultrafast dynamics research by offering fully coherent ultrabright femtosecond X-ray pulses. The cutting-edge technology developed around the XFELs has enabled revolutionary breakthroughs in multiple disciplines in the past decade. X-ray emission/absorption spectroscopy, X-ray scattering, and X-ray crystallography have quickly adapted to the XFEL facilities, investigating high-resolution structure and dynamics. The development of the XFEL-based time-resolved methods is particularly significant for light-sensitive macromolecules. Novel insights into the structural dynamics are being gathered for a comprehensive understanding of the detailed process and its underlying molecular mechanism.

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Remote Molecular Modulation in Polariton Chemistry

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Keywords: Light-matter strong coupling, Ultrafast infrared spectroscopy, Optical cavity, Polariton chemistry

Abstract: The emergence of molecular vibrational polaritons (MVPs) has largely centered on reports of ground-state reactivity changes[1] under vibrational strong coupling (VSC) regime. Yet, such effects appear largely system-dependent and a broadly accepted mechanism remains unclear. In parallel, ultrafast spectroscopy provides multidimensional views of hybrid light–matter systems[2,3]. In this talk, the combinations of tailored cavity architectures and spectroscopic techniques will be demonstrated to show how polaritonic and non-polaritonic chemistries can be remotely unified within a single framework. These results would suggest practical design rules for controlling reactivity via MVPs beyond the conventional strong-coupling paradigm on both ground and optically excited states.

References

1. Thomas A, and Ebbesen T, et al. *Angewandte Chemie*, 2016, 128.38, 11634-11638.
2. Xiang B, and Xiong W, et al. *Science advances*, 2021, 7.19, eabf6397.
3. Xiang B, and Xiong W, et al. *Advanced Optical Materials*, 2022, 10.5, 2102237.

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Photoexcitation Dynamics in Condensed-Phase Materials

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Keywords: Photoexcitation charge and spin dynamics, electron-phonon and spin-orbit coupling, Coulomb interaction, nonadiabatic molecular dynamics, time-dependent density functional theory

Abstract: Nonadiabatic effects strongly shape excited-state dynamics and play a key role in photophysical and photochemical processes. This talk examines how multiple degrees of freedom—including electron–phonon coupling, spin–orbit coupling, Coulomb interactions, and photon–exciton–phonon coupling—jointly govern the evolution of charges, spins, and polaritons across several representative material systems.[1-3] By integrating these couplings within a unified dynamical framework, we reconcile long-standing discrepancies between experiment and theory and reveal a coherent, hierarchy-resolved mechanistic picture. The resulting insights provide a solid physical foundation for understanding excited-state phenomena dominated by nonadiabatic effects.

References

1. R. Lu, Run Long, *Nano Lett.* 2024, 24, 8970-8947.
2. S. Shen, H. Lu, S. Gumber, O. V. Prezhdo, R. Long, *Nano Lett*. 2025, 25, 7517-7523.
3. X. Xu, X. Han, E. Stippell, W. Fang, O. V. Prezhdo, R. Long, *Nano Lett*. 2025, 25, 13063-13069.

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