



第八届亚洲分子光谱研讨会

The 8th Asian Workshop on Molecular Spectroscopy

会议手册

主办单位: 吉林大学

承办单位: 吉林大学化学学院 长春理工大学化学与环境工程学院

吉林大学理论化学研究所 吉林大学超分子结构与材料国家重点实验室

吉林省光功能材料与化学国际联合研究中心

2024年9月11日-14日 中国·长春

September 11 to 14, 2024 ChangChun · China



吉林大学

8th AWMs



ChangChun · China

DIRECTORY

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The 8th Asian Workshop on Molecular Spectroscopy**Introduction**

Building on the remarkable achievements of previous workshops, we will be holding the 8th Asian Workshop on Molecular Spectroscopy in Changchun (Jilin, China) on September 11 to 14, 2024. The AWMS is committed to promoting academic exchanges between experimental and theoretical researchers in the field of molecular spectroscopy from all over the world, especially encouraging young scientists to present their latest work. The upcoming 8th AWMS will feature 8 topics and host 4 plenary speakers and about 30 invited speakers. We warmly invite researchers and students to participate in this conference, where you will have the chance to engage with peers, gain new insights, and contribute to the development of molecular spectroscopy.

The themes that we intend to cover in this meeting are as follows:

- Spectroscopy in gas phase
- Application of spectroscopy to dynamics
- New spectroscopic techniques
- Precision measurement
- Theoretical analysis
- Spectroscopy of condensed phase/solid
- AI for spectroscopy
- Atmospheric and interstellar spectra
- Other topics

Date

Date of conference: September 12 to 14, 2024

Date of arrival: September 11

Date of departure: September 15

Venue

Qianwei Campus South Area of Jilin University, ChangChun, China.

Homepage

<https://awms-meeting.org/index.html>

Registration and Payment

<https://awms-meeting.org/Registration.html>

Abstract Submission

1. The submitted abstract should follow the workshop website's template and be one page in length.
2. Before sending in your abstract online via the workshop website, please review the requirements on the submission page.
3. The conference will include plenary and invited lectures, oral representations, and poster sessions.
4. A poster with a resolution of at least 300 dpi and dimensions of 90 by 120 cm is advised. Free printing will be offered for posters submitted to AWMS2024@jlu.edu.cn by August 30th.
5. Abstract submission deadline is August 15, 2024.

Plenary speakers

Minhaeng Cho	Korea University
Yunjie Xu	University of Alberta
Tomonari Wakabayashi	Kindai University
Yi Luo	University of Science and Technology of China

Confirmed Invited Speakers/Chairs

Masaaki Baba	Kobe University
Evan Bieske	The University of Melbourne
Yasuki Endo	Yang Ming Chiao Tung University
Feng Gai	Peking University
Hong Gao	Institute of Chemistry, Chinese Academy of Sciences
Qian Gou	Chongqing University
Jens-Uwe Grabow	Leibniz Universität Hannover
Tsuneo Hirano	Ochanomizu University
Gao-Lei Hou	Xi'an Jiaotong University
Shuiming Hu	University of Science and Technology of China
Wolfgang Jäger	University of Alberta
Zhenggang Lan	South China Normal University
Hui Li	Jilin University
Anwen Liu	University of Science and Technology of China
Jian Liu	Peking University
Zhi-Heng Loh	Nanyang Technological University

Jun Miyazaki Tokyo Denki University
Eli Pollak Weizmann Institute of Science
Paul L. Raston University of Hawai'i at Mānoa
Zefeng Ren Dalian Institute of Chemical Physics, Chinese Academy of Sciences
Timothy Schmidt University of New South Wales
Thomas Schultz Ulsan National Institute of Science and Technology
Germán Sciaini University of Waterloo
Jian Tang Okayama University
Masashi Tsuge Hokkaido University
Hongfei Wang Westlake University
Yuxiang Weng Institute of Physics, Chinese Academy of Science
Andong Xia Beijing University of Posts and Telecommunications
Daiqian Xie Nanjing University
Chang Yan Shanghai Jiao Tong University
Qin Yang Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences
Yanqiang Yang Institute of Fluid Physics, China Academy of Engineering Physics
Chunfeng Zhang Nanjing University
Wenkai Zhang Beijing Normal University
Zhen Zhang Institute of Chemistry, Chinese Academy of Sciences
Dongping Zhong Shanghai Jiao Tong University
Mingfei Zhou Fudan University
Wei Zhuang Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences

Conference Chairs

Shuiming Hu University of Science and Technology of China
Hui Li Jilin University

Committees**International Committees**

Masaaki Baba Kobe University
Qian Gou Chongqing University

Jens Uwe Grabow Leibniz Universität Hannover
Gaolei Hou Xi'an Jiaotong University
Yen Chu Hsu Central University
Shuiming Hu University of Science and Technology of China
Jer Lai Kuo Institute of Atomic and Molecular Sciences, Taiwan Academia Sinica
Chan Ho Kwon Kangwon National University
Sang Kuk Lee Pusan National University
Yuan Pern Lee Yang Ming Chiao Tung University
Hui Li Jilin University
Anwen Liu University of Science and Technology of China
Jun Miyazaki Tokyo Denki University
Thomas Schultz Ulsan National Institute of Science and Technology
Jian Tang Okayama University
Kaito Takahashi Institute of Atomic and Molecular Sciences, Taiwan Academia Sinica
Masashi Tsuge Hokkaido University

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General Program

Date	Time	Event	Location
Sep 11	10:00-22:00	Registration	Dong Fang Yue Hua Hotel or Lavande Hotel
	18:00-20:00	Dinner	Dong Fang Yue Hua Hotel
Sep 12	08:00-08:20	Opening Ceremony	Circular Lecture Hall, second floor, Inorganic-Supramolecular Building
	08:20-12:25	Lectures	
	12:25-13:30	Lunch	Hu Pan Restaurant
	13:30-18:00	Lectures	Circular Lecture Hall, second floor, Inorganic-Supramolecular Building
	18:00-19:30	Dinner	Hu Pan Restaurant
Sep 13	08:30-12:25	Lectures	Circular Lecture Hall, second floor, Inorganic-Supramolecular Building
	12:20-13:05	Lunch	Hu Pan Restaurant
	13:05-14:05	Poster Presentation	Circular Lecture Hall, second floor, Inorganic-Supramolecular Building
	14:05-18:05	Lectures	Circular Lecture Hall, second floor, Inorganic-Supramolecular Building
	18:05-19:00	Dinner	You Yi Hall
Sep 14	08:30-12:15	Lectures	Circular Lecture Hall, second floor, Inorganic-Supramolecular Building
	12:15-12:30	Award and Closing Ceremony	
	12:30-13:30	Lunch	Hu Pan Restaurant
	14:00-18:00	City Tour	Jingyuetan National Scenic Area

Schedule

Sep. 12				
Events	Time	Name/ Affiliation	Title	Chair
08:00-08:20 Opening Ceremony				
Plenary	08:20-08:55	Minhaeng Cho/ Korea University	Frequency comb nonlinear spectroscopy: From single photon interferometry to multidimensional spectroscopy	Hongfei Wang Eli Pollak
Invited	08:55-09:20	Feng Gai/ Peking University	Site-Specific Assessment of the Structure and Dynamics of Amyloid Fibrils	
Invited	09:20-09:45	Germán Sciaini/ University of Waterloo	WaterFEL: Advancing Molecular Spectroscopy and Diffraction with Cutting-Edge Electron Based Methods	
Invited	09:45-10:10	Wenkai Zhang/ Beijing Normal University	Femtosecond optics and X ray lasers study of chloride pumped rhodopsin	
10:10-10:40 Photo Session, Break & Communication				
Invited	10:40-11:05	Hongfei Wang/ Westlake University	Surface for spectroscopy: selection rules and question on the vibrational normal mode	Minhaeng Cho Yi Luo
Invited	11:05-11:30	Zefeng Ren/ Dalian Institute of Chemical Physics, Chinese Academy of Sciences	Probing the ¹ (TT) State of TIPS-Pentacene by Heterodyne-detected Sum Frequency Generation Electronic Spectroscopy	
Invited	11:30-11:55	Zhenggang Lan/ South China Normal University	Nonadiabatic Dynamics and Time-Resolved Pump Probe Spectra	
Oral	11:55-12:10	Yangyang Zeng/ Institute of Fluid Physics, China Academy of Engineering Physics	Investigation of Structures, Vibrational Dynamics, Phase Transitions of Energetic Materials using Mid- and Far- Infrared Spectroscopy	
Oral	12:10-12:25	Xin-Xing Zhang/ Dalian University of Technology	Mechanism and Regulation of Metal Ion-Induced Phase Separation in Peptide Solutions	
12:25-13:30 Lunch				

Events	Time	Name/ Affiliation	Title	Chair
Plenary	13:30-14:05	Yi Luo/ University of Science and Technology of China	A generalized theoretical approach for molecular response under a highly confined electromagnetic field	Thomas Schultz Daiqian Xie
Invited	14:05-14:30	Zhi-Heng Loh / Nanyang Technological University	Capturing Transient Species in Ionized Liquid Water	
Invited	14:30-14:55	Eli Pollak/ Weizmann Institute of Science	Vibrational perturbation theory for energy splitting in symmetric double well potentials	
Invited	14:55-15:20	Chunfeng Zhang/ Nanjing University	Excited-State Dynamics in Organic Photovoltaic Systems under Solar Light Equivalent Excitation	
Invited	15:20-15:45	Qin Yang/ Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences	The Role of Electronic Structure Calculation Methods and Solvent Models in Anharmonic Simulation of Chiral Vibrational Spectra	
15:45-16:05 Break & Communication				
Invited	16:05-16:30	Yuxiang Weng / Institute of Physics, Chinese Academy of Science	Quantum Phase Synchronization via Exciton-Vibrational Energy Dissipation Sustains Long lived Coherence in Photosynthetic Antennas	Feng Gai Anwen Liu
Invited	16:30-16:55	Jian Liu/ Peking University	Nonadiabatic Field Approaches for Electronic and Vibrational Spectra	
Invited	16:55-17:20	Timothy Schmidt/ University of New South Wales	Intermediates in Singlet Fission and Triplet Fusion	
Invited	17:20-17:45	Wei Zhuang/ Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences	Towards Understanding the Mechanism of the Ultrafast Dynamics of Water Hydrogen Bonding Network In Bulk and Interfaces	
Oral	17:45-18:00	Jiwen Jian/ Zhejiang Normal University	Spectroscopic identification of two Be ₂ -benzene species featuring Be-Be single bond and pseudo-triple bond	

Sep. 13				
Events	Time	Name/ Affiliation	Title	Chair
08:00-08:20 Opening Ceremony				
Plenary	08:30-09:05	Tomonari Wakabayashi/ Kindai University	Laboratory Measurements and Theoretical Simulations of Infrared Emission Spectra of Fullerene C ₆₀	Shuiming Hu Yunjie Xu
Invited	09:05-09:30	Paul L. Raston/ University of Hawai'i at Mānoa	Broadband Microwave Spectroscopy of Asymmetric Top Molecules Solvated with Helium Atoms	
Invited	09:30-09:55	Tsuneo Hirano/ Ochanomizu University	Schrödinger's Cat and Molecular Spectroscopy: Vibrationally Averaged Structures of linear Molecules	
Invited	09:55-10:20	Gao-Lei Hou/ Xi'an Jiaotong University	Infrared Spectroscopy of Fullerene-metal Complexes and Their Potential Cosmic Relevance	
10:20-10:40 Break & Communication				
Invited	10:40-11:05	Mingfei Zhou/ Fudan University	Heavy-Atom Tunneling Reactions in Cryogenic Matrices	Wolfgang Jäger Tomonari Wakabayashi
Invited	11:05-11:30	Masaaki Baba/ Kobe University	Benzene is observed as being bent out-of-plane: No molecule is observed as it is in the equilibrium structure	
Invited	11:30-11:55	Hui Li/ Jilin University	Full dimensional intermolecular potential energy surface construction and spectroscopic calculation for van der Waals complexes	
Oral	11:55-12:10	Ziqiu Chen/ Lanzhou University	Pure rotational and rovibrational spectroscopy of cyclopropylamine in the far-infrared region: Probing the conformational isomerism	
Oral	12:10-12:25	Yilang Liu/ Nanjing University	Analyzing Multi-channel Shape Resonances in Cold Collisions through Wavefunctions	
12:25-13:05 Lunch				
13:05-14:05 Poster Presentation				

Events	Time	Name/ Affiliation	Title	Chair
Invited	14:05-14:30	Wolfgang Jäger/ University of Alberta	Rotational Spectroscopy of Complexes and Clusters: From Pure Dispersion to Hydrogen Bond Dominated Interactions	Yasuki Endo Masaaki Baba
Invited	14:30-14:55	Jian Tang/ Okayama University	Infrared Spectroscopy of the NO ₃ Radical	
Invited	14:55-15:20	Hong Gao/ Institute of Chemistry, Chinese Academy of Sciences	Spectroscopic and photodissociation study of C ₂ in vacuum ultraviolet region	
Invited	15:20-15:45	Jun Miyazaki/ Tokyo Denki University	Density Functional Theoretical Study of Tris (cyclopentadienyl) lanthanide in Solid Argon Matrices	
15:45-16:05 Break & Communication				
Invited	16:05-16:30	Yasuki Endo/ Yang Ming Chiao Tung University	FTMW spectroscopy of chlorine bearing free radicals	Mingfei Zhou Jian Tang
Invited	16:30-16:55	Evan Bieske/ The University of Melbourne	Spectroscopy of Carbon Cluster Cations in the Gas Phase	
Invited	16:55-17:20	Masashi Tsuge/ Hokkaido University	Physicochemical behavior of radicals adsorbed on ice: Application of REMPI method for in situ detection	
Oral	17:20-17:35	Zhen-Dong Sun/ Shandong University	Adsorption Configurations and Interaction Behaviors of CO and CO ₂ on CoO(001) Surfaces Probed by UHV-PR-FTIRs	
Oral	17:35-17:50	Yan Tan/ University of Science and Technology of China	Line intensity measurement of CO and H ₂ transitions with 0.1% precision	
Oral	17:50-18:05	Jiahui Xiong/ Toyama University	New A ² Π -X ² Σ ⁺ Bands of CaH	

Sep. 14				
Events	Time	Name/ Affiliation	Title	Chair
Plenary	08:30-09:05	Yunjie Xu/ University of Alberta	Unlocking the Mysteries of Chiral Phenomena in Complex Environments: A Multifaceted Chiral Spectroscopic Approach	Jens-Uwe Grabow Yanqiang Yang
Invited	09:05-09:30	Dongping Zhong/ Shanghai Jiao Tong University	Optical Coherent Control of Molecular Reactions in Chemistry and Biology	
Invited	09:30-09:55	Zhen Zhang/ Institute of Chemistry, Chinese Academy of Sciences	Nonlinear Spectroscopic Investigation of Supramolecular Chiral Self Assembly and Dynamics at Interfaces	
Invited	09:55-10:20	Qian Gou/ Chongqing University	Rotational Insights into Binding and Aggregation Behaviors of Carbon Dioxide	
10:20-10:40 Break & Communication				
Invited	10:40-11:05	Jens-Uwe Grabow/ Leibniz Universität Hannover	Passaging And Resonant Impulse Synergy -Rotational electric resonance by chirp and single-tone excitation of supersonic jets: PARIS	Dongping Zhong Germán Sciaini
Invited	11:05-11:30	Chang Yan/ Shanghai Jiao Tong University	Multidimensional Widefield Infrared-Encoded Spontaneous Emission (MD-WISE) Microscopy: Distinguishing Chromophores by Ultrashort Infrared Pulses	
Oral	11:30-11:45	Chuanxi Duan/ Central China Normal University	High resolution infrared spectra of formic acid dimer and trimer	
Oral	11:45-12:00	Gang Feng/ Chongqing University	Rotational Spectroscopic Investigation of the Thiol Benzofuran Complexes: the Synergistic Role of S-H···π, S-H···O and C-H···π Interactions	
Oral	12:00-12:15	You-Liang Zhu/ Jilin University	A molecular dynamics simulation software for polymers	
12:15-12:30 Award and Closing Ceremony				
14:00- City Tour				

Abstract Contents

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02. Yi Luo A generalized theoretical approach for molecular response under a highly confined electromagnetic field
03. Yunjie Xu Unlocking the Mysteries of Chiral Phenomena in Complex Environments: A Multifaceted Chiral Spectroscopic Approach
04. Tomonari Wakabayashi Laboratory Measurements and Theoretical Simulations of Infrared Emission Spectra of Fullerene C60
05. Masaaki Baba Benzene is observed as being bent out-of-plane: No molecule is observed as it is in the equilibrium structure.
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11. Jens-Uwe Grabow Passaging And Resonant Impulse Synergy -Rotational electric resonance by chirp and single-tone excitation of supersonic jets: PARIS
12. Tsuneo Hirano Schrödinger's Cat and Molecular Spectroscopy: Vibrationally Averaged Structures of linear Molecules
13. Gao-Lei Hou Infrared Spectroscopy of Fullerene-metal Complexes and Their Potential Cosmic Relevance
14. Wolfgang Jäger Rotational Spectroscopy of Complexes and Clusters: From Pure Dispersion to Hydrogen Bond Dominated Interactions
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21. Zefeng Ren Probing the 1(TT) State of TIPS-Pentacene by Heterodyne-detected Sum Frequency Generation Electronic Spectroscopy
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23. Germán Sciaini WaterFEL: Advancing Molecular Spectroscopy and Diffraction with Cutting-Edge Electron-Based Methods
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28. Andong Xia Probing the Effect of Solvation of Excited State Molecules
29. Chang Yan Multidimensional Widefield Infrared-Encoded Spontaneous Emission (MD-WISE) Microscopy: Distinguishing Chromophores by Ultrashort Infrared Pulses
30. Qin Yang The Role of Electronic Structure Calculation Methods and Solvent Models in Anharmonic Simulation of Chiral Vibrational Spectra.
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43. Yan Tan Line intensity measurement of CO and H2 transitions with 0.1% precision
44. Jiahui Xiong New A² Π -X² Σ^+ Bands of CaH
45. Yangyang Zeng Investigation of Structures, Vibrational Dynamics, Phase Transitions of Energetic Materials using Mid- and Far- Infrared Spectroscopy

46. Xin-Xing Zhang Mechanism and Regulation of Metal Ion-Induced Phase Separation in Peptide Solutions
47. You-Liang Zhu A molecular dynamics simulation software for polymers
48. Fanghui Cao Precision spectral measurement of methane in the 2v₃ transition band
49. Xiumian Cao An Atomic Force Microscopy and Total Internal Reflection Fluorescence Microscopy Correlated System (AFM-TIRF) for Fluorescence Imaging and Spectroscopy of a Single Particle
50. Lili Cong Microfluidic Droplet-SERS Platform for Single-Cell Cytokine Analysis via a Cell Surface Bioconjugation Strategy
51. Wenji Jiang SERS/UV-vis analyzes the heterogeneous photocatalytic degradation
52. Meiyue Li Probing Pre-Reaction Intermediates for Ring-Opening Reactions between Epoxides and Acids
53. Zihui Liang Research on Metasurface Regulated Electrochemiluminescence Strategy for Exosome Detection
54. Di Liu Multienzyme-like aerogel as SERS/colorimetric sensing platform for the fermentation process of tea
55. Jia Liu Revealing the ultrafast energy transfer pathways in energetic materials: Time-dependent and quantum state-resolved
56. Jiaqi Lu Optical Photothermal Infrared (O-PTIR) Spectroscopic Analysis of Cryptochrome CRY2 protein for its Blue Light-induced Phase Separation Phenomenon
57. Ziwen Ma In situ Synchronization Single Molecule Force-Infrared Spectroscopy Characterizing of Mechanochemistry
58. Ming Mu Surface enhanced Raman spectroscopy research on self-supporting MIL-100(Fe)/AgCl/Ag
59. Jia Nie Two-dimensional sum frequency generation spectra simulation of the water interface based on local quantum vibration embedding to reveal hydrogen bond dynamics at water interfaces
60. Lijia Shang Surface-enhanced Raman scattering of Polyoxometalate-Based Metal Organic Frameworks
61. Yunfei Song Application of fs-CARS Technology in Combustion Diagnostics
62. Ruonan Teng Synthesis of Aluminium-doped Zinc Oxide Nanomaterials and Atmospheric Window Emissivity Studies in the Infrared Region
63. Qing Tian Micromodulation of methyl formate by supercritical carbon dioxide extraction
64. Jiaqi Wang Surface-Enhanced Raman Scattering and Machine Learning Technique Used for Disease Identification
65. Mengmeng Wang Two types of water at the poly(methyl methacrylate)/water interface revealed by Time-Resolved Sum-Frequency Generation Vibrational Spectroscopy
66. Sisi Wen Construction of two-dimensional metal sulfide-based nanozyme-SERS substrates
67. Haosen Xu SERS-based Au@CDs with SOD activity for free radical scavenging
68. Yumei Yang Synergistic enhancement of ultrahigh SERS activity via Cu₂O@C/Ag yolk shell structure with different cavity thickness
69. Zitong Yu Revealing intracellular lipid droplet microenvironment in pathophysiological events by two-photon fluorescence spectroscopy
70. Bo-Jun Zhao Time and Frequency Resolved Infrared Free Induction Decay (IR-FID) of Atmospheric H₂O Observed in Surface Sum-Frequency Generation Vibrational Spectroscopy (SFG-VS)
71. Menghan Zhao The Au@RCDs with core-shell structures were used for in situ SERS detection in biological systems
72. Yonglong Zhang Insights on Z-scheme interfacial charge transfer of TiO₂-NRAs/BiOI-NFs/ Au-NPs nanoheterostructures and unveiling enhanced photoelectrochemical performances
73. Xiaoxuan Zheng Local Electric Field in Nanocavities Dictates the Vibrational Relaxation Dynamics of Interfacial Molecules
74. Zhaoyang Zheng Vibration Excitation Dynamics in Nitromethane by First-Principles Molecular Dynamics Simulations
75. Jinyu Zhu In Situ Raman Spectroscopy Reveals Cytochrome c Redox Controlled Modulation of Mitochondrial Membrane Permeabilization That Triggers Apoptosis

Abstract**Frequency comb nonlinear spectroscopy: From single photon interferometry to multidimensional spectroscopy****Minhaeng Cho^{1,2}**¹*Center for Molecular Spectroscopy and Dynamics (CMSD), Institute for Basic Science (IBS), Seoul 02841, Republic of Korea*²*Department of Chemistry, Korea University, Seoul 02841, Republic of Korea*

In spectroscopy, researchers frequently encounter a dilemma when the tool they employ for observation – light – also triggers alterations in their target materials and molecular systems. This problem is particularly pronounced for ultrafast spectroscopy methods, where prolonged exposure to high-energy laser light is imperative to capture subtle and weak nonlinear responses. This necessity poses a difficulty, particularly when dealing with materials that lack the photostability required by conventional spectroscopic approaches. This situation underscores the challenge: the acquisition of data under such circumstances becomes demanding and, at times, seemingly impossible. Therefore, the reduction of data acquisition time is essential when the observed materials deviate from established photostability standards. Over the past years, we developed asynchronous and interferometric (AI) transient absorption (TA) and two-dimensional electronic spectroscopy (2DES) techniques based on (i) asynchronous sampling for an automatic pump-probe delay generation and (ii) interferometric detection of the nonlinear optical spectrum without using spectrograph and array detectors. The AI-TA and AI-2DES enable ultrafast dynamics measurements in seconds due to their rapid data acquisition capability. We have demonstrated that AI nonlinear spectroscopy utilizing two repetition-frequency-stabilized and synchronized mode-locked lasers can be of great use for investigating ultrafast dynamics in semiconducting materials such as Te microcrystals and perovskite nanocrystals and light-harvesting complexes. In addition, if time permits, I would like to discuss our experimental results on frequency comb single-photon interferometry. By using a frequency comb laser and two stimulated parametric downconversion processes, we generated signal photons at the single-photon level. Our findings provide deeper insights into the environmental effects on wave-particle duality in quantum mechanics and pave the way for developing remote quantum spectroscopy with undetected photons.

A generalized theoretical approach for molecular response under a highly confined electromagnetic field

Yi Luo

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The creation of plasmonic nanocavity provides a powerful tool to break the conventional diffraction limit of light, enabling to experimentally achieve ultrahigh spatial resolution of molecular Raman image. The strong spatial confinement effect of plasmonic field has challenged the conventional molecular response theory, as widely adopted plan wave approximation for the light is no longer applicable. In this talk, I will briefly introduce our generalized molecular response theory in the framework of effective field Hamiltonian (EFH), which allows to effectively take all characteristics of localized plasmonic fields into consideration. In combination with first principles simulations, it can quantitatively reproduce state-of-the-art experimental observations, revealing the underlying intrinsic physics and mechanisms. The predictive power of EFH is demonstrated by several new phenomena generated from its peculiar spatial, momentum, time, and energy structures. The corresponding experimental verifications are also briefly described. Finally, I will also briefly discuss the possibility of building large spectroscopy model in the era of artificial intelligence.

Unlocking the Mysteries of Chiral Phenomena in Complex Environments:

A Multifaceted Chiral Spectroscopic Approach

Yunjie Xu

Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada, T6G 2G2

Our research program centers on unraveling mechanisms of chirality recognition, transfer, amplification at the molecular level. To achieve this, we explore chirality-related properties of systems across a spectrum of size regimes, encompassing small chiral molecules to atomically precise metal clusters, nanoparticles, and crystals. Our investigations traverse diverse environments, from the gas phase to solution environments and liquid-liquid interfaces. By emphasizing the interplay among different size scales, we aim to extract new physical insights into these intricate chirality events.

While conducting Raman optical activity (ROA) measurements of several transition metal complexes under near resonance condition, we detected very strong chiral Raman signals of achiral solvents. Our search for possible mechanisms led to the discovery of a new form of chiral Raman spectroscopy called eCP-Raman, which combines electronic circular dichroism and circularly polarized Raman (CP-Raman) into one.¹ Building on this discovery, our recent efforts focused on deciphering the chiral spectral features at the luminescence bands of europium complexes using an ROA instrument, where we uncovered multiple contributions to the observed signals. Next, I will present vibrational circular dichroism investigations on atomically precise chiral silver clusters where strong exciton couplets were detected. By utilizing simulations of the full metal clusters, we extracted some intriguing structural details of these metal clusters and explored bi-directional chirality transfer events between the chiral ligands and the metal cores. If time permits, I will discuss our recent efforts in using a genetic algorithm to assign VCD features of two Salen ligands in order to uncover their dominant conformations in solution.

¹ G. Li, M. Alshalalfeh, J. Kapitán, P. Bouř, Y. Xu, *Eur. J. Chem.* **2022**, 28, e202104302; G. Li, M. Alshalalfeh, Y. Yang, J. R. Cheeseman, P. Bouř, Y. Xu, *Angew. Chem. Int. Ed.* **2021**, 60, 22004; T. Wu, G. Li, J. Kapitán, J. Kessler, Y. Xu, P. Bouř, *Angew. Chem. Int. Ed.* **2020**, 59, 21895; -21898; G. Li, J. Kessler, J. Cheramy, T. Wu, M. R. Poopari, P. Bouř, Y. Xu, *Angew. Chem. Int. Ed.* **2019**, 58, 16495.

Laboratory Measurements and Theoretical Simulations of Infrared Emission Spectra of Fullerene C₆₀

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Fullerene C₆₀ is known for its highly symmetric icosahedral molecular structure [1]. Among the total 46 distinct normal modes of vibration, only four modes of T_{1u} symmetry are infrared (IR) active, as evidenced for the presence of C₆₀ in the laboratory produced carbon soot [2]. The C₆₀ and C₇₀ molecules were detected in a protoplanetary nebula by their IR emission spectra using the satellite observatory, Spitzer IRS [3]. The molecular IR emission of C₆₀ has been observed in many objects in the late stages of the stellar evolution and the excitation mechanism of C₆₀ in space as well as the formation mechanism are under debate [4]. For astrophysical implications of the abundance of C₆₀ in space, we measured IR emission spectra of C₆₀ thin films and simulated the spectra at elevated temperatures [5].

Figure 1 shows a typical IR emission spectrum of the C₆₀ thin film with 0.54- μ m thickness at 362 K. Four bands are conspicuous at 526, 575, 1182, and 1427 cm⁻¹ for the T_{1u} modes. Figure 2 plots simulated temperature dependence of the IR emission band intensity of the four T_{1u} modes of C₆₀ for which all the fundamentals, overtones, and combinations up to the excitation by seven vibrational quanta are taken into considerations. Low-frequency modes of T_{1u}(1) and T_{1u}(2) have substantial intensity above 100 K, whereas high-frequency modes of T_{1u}(3) and T_{1u}(4) appear above 200 K. The difference of onsets is explainable by the different thermal population in vibrationally excited states for relevant modes of distinctly different vibrational frequencies. We will discuss how and why the IR emission spectrum of an ensemble C₆₀ molecules changes with temperature.

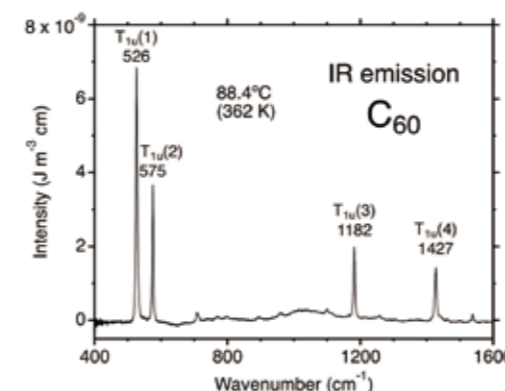


Fig. 1: IR emission spectra of the fullerene C₆₀ thin film at 88.4°C (362 K).

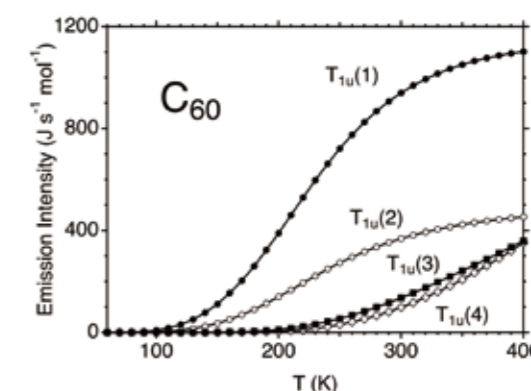


Fig. 2: Simulated temperature dependence of the emission band intensity of the four T_{1u} modes of C₆₀ [5].

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Benzene is observed as being bent out-of-plane:

No molecule is observed as it is in the equilibrium structure.

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Kunishige et al. have accurately determined rotational constants of benzenes for all deuterium isotopologues by ultrahigh-resolution laser spectroscopy and concluded that the averaged bond lengths $r_0(\text{C-H})$ and $r_0(\text{C-D})$ are almost identical [1] contrary to the believed general rule that $r_0(\text{C-D})$ is generally shorter than $r_0(\text{C-H})$ because of anharmonicity in the potential energy curve of stretching vibration.

In order to explain this experimental result, we considered that the expectation value of C-H out-of-plane bending vibration angle is not zero (Fig. 1), and the bond lengths projected to the molecular plane (inertial principal axis) $r_{0,\text{proj}}(\text{C-H})$ and $r_{0,\text{proj}}(\text{C-D})$ become almost identical, because the $r_0(\text{C-H})$ is larger but the bending angle is also larger (Fig. 2). The apparent reduction of averaged bond length cancels the difference in the effective bond length between $r_{0,\text{proj}}(\text{C-H})$ and $r_{0,\text{proj}}(\text{C-D})$ [2].

It indicates that the benzene molecule is observed as being bent out of plane. It can be understood by considering the pendulum motion, in which the existence probability is large at the turning point. We also performed theoretical calculations of path integral molecular dynamics and found that most of all benzene molecules are nonflat with various shapes and the average out-of-plane angle was approximately 6 degrees [3].

It is essential to perform accurate theoretical calculation and reconsider the experimental results of rotational constant, intensity of vibrational transition, electron diffraction, and so on.

No molecule is observed as it is in the equilibrium structure. In deriving molecular structure from the observed effective rotational constants, we must keep in mind how the molecule was recognized on the observation.

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Indicate your choice :

Oral Presentation

Poster Presentation

Spectroscopy of Carbon Cluster Cations in the Gas Phase

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Carbon clusters are produced in flames and discharges and are present in various interstellar environments (protoplanetary disks, nebulae, interstellar space). Laboratory infrared and electronic spectra are essential for the remote detection of carbon clusters and for understanding their structures. However, obtaining and interpreting carbon cluster spectra are complicated by the presence of different isomers. For example, the C_{36}^+ cation has fullerene, ring, and bi-ring isomers whose spectra must be disentangled. In order to address spectroscopic ambiguities associated multiple isomers, we have adopted a strategy whereby the charged clusters are separated in an ion mobility stage before mass-selection and spectroscopic interrogation in a cryogenically cooled ion trap.¹⁻³ The instrument allows us to select a particular C_n^+ isomer produced by the laser ablation ion source (see Figure 1) and probe it using tunable laser radiation. We will present and discuss electronic and infrared spectra of bare carbon clusters, and also carbon clusters that have been hydrogenated or oxygenated, highlighting their possible astrophysical relevance.

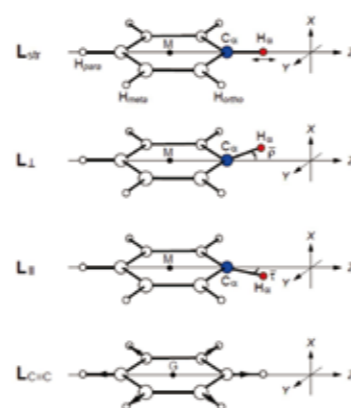


Fig. 1 C-H and C-C vibration of benzene

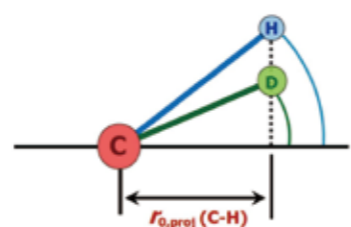


Fig. 2 Projection of C-H(D) bond to the molecular plane

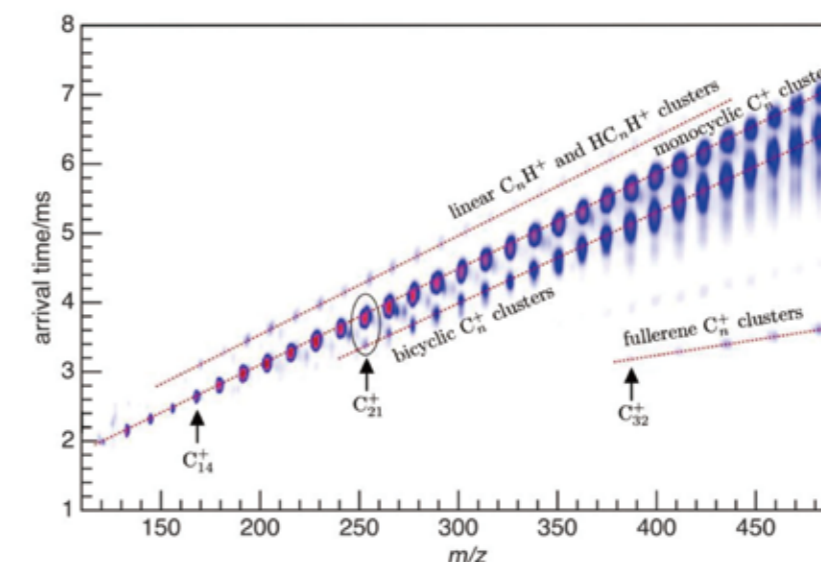


Fig. 1: Plot of ion signal as a function of m/z and drift time, showing C_n^+ families associated with cyclic, bi-cyclic and fullerene clusters.

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FTMW spectroscopy of chlorine bearing free radicals

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Free radicals containing a chlorine atom are playing important roles in atmospheric chemistry. For example, the ClO radical is known to play important roles in the ozone layer depletion in the stratosphere. Not only limited to chemistry in the stratosphere, they also play important roles in the troposphere. Recently, we have observed several chlorine bearing free radicals by FTMW spectroscopy. We will present some of the results obtained in the recent works.

The ClSO and ClSS radicals are members of XOO, XSO, XSS radicals where X denotes H, F, and Cl. High resolution spectroscopic studies have been reported for most of this series of radicals, where, however, high resolution spectroscopic studies of ClSO are missing. For ClSS, although mm- and submm-wave spectroscopy has been reported, no gas phase study resolving its hyperfine structure has been reported before. We have observed their pure rotational spectra in the cm-wave region and have determined precise molecular constants including their fine and hyperfine interaction constants[1]. All of this series of radicals have known to have $^2A'$ ground state, and have similarities. However, it was found that FOO and ClOO are quite different from other related species.

We also have observed pure rotational spectra of the ClCO radical. Unlike the ClSO and ClSS radicals, it has the $^2A'$ ground electronic state and fairly large ClCO angle with the rotational constant A to be about 156 GHz. We were able to observe only $K_a = 0$, a -type transitions. Thus, a limited number of molecular constants were determined for this radical.

The ClC(O)OO radical is considered to be an O₂ adduct of ClCO, and two conformers, *trans*-ClC(O)OO and *cis*-ClC(O)OO are expected as shown in Fig. 1. Although the *cis*-conformer is about 3 kJ/mol higher in energy, spectra of both of the conformers were observed with similar intensities. Molecular constants including the fine and hyperfine interaction constants were determined precisely for ³⁵Cl and ³⁷Cl isotopologues. The determined constants shows that the unpaired electron is mainly localized on the terminal oxygen, with the $^2A'$ ground state.

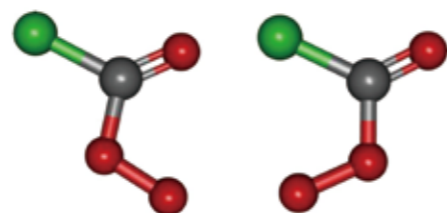


Fig. 1 Two conformers of ClC(O)OO, (left) *trans*- and (right) *cis*-conformers.

Rotational spectra of one isomer of the chlorovinoxy radical, *trans*-CHClCHO were observed. We were able to observe a -type transitions with $K_a = 0$ and 1. Although we used *trans*-1,2-dichloroethylene and *cis*-1,2-dichloroethylene with oxygen diluted in Ar or Ne as precursors, only the *trans*-isomer were observed, where both of the isomers are separated by a fairly high barrier and *cis*-isomer is only 4.9 kJ/mole higher in energy.

Reference:

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Site-Specific Assessment of the Structure and Dynamics of Amyloid Fibrils

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Many spectroscopic techniques, such as infrared (IR) spectroscopy and fluorescence spectroscopy, are widely used in biological sciences. However, most biological systems lack an intrinsic and suitable molecular signal that can be used to extract site-specific chemical or physical information of interest via spectroscopic measurement and hence require labeling of an external reporter that bears desired spectroscopic property. In this regard, unnatural amino acid-based (UAA-based) spectroscopic probes have recently gained popularity in the study of the structure, dynamics, hydration, and electrostatics of proteins in a site-specific manner. In this talk, we will focus on discussing the application of UAA-based IR probes to site-specifically interrogate the local structure and hydrogen-bonding (H-bonding) dynamics of amyloid fibrils, as well as the effect of dehydration on the kinetics and mechanism of amyloid fibril formation.

Spectroscopic and photodissociation study of C₂ in vacuum ultraviolet region

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The dicarbon molecule, C₂, has been widely observed in various energetic environments, like flames, carbon stars, interstellar medium, comets and so on. Spectroscopic studies of C₂ and identifications of the corresponding electronic transitions can be dated back to 19th century [1]. Most of the previous studies have been limited to relatively low energy region, spectroscopic and photodissociation investigations of C₂ in vacuum ultraviolet (VUV) have been rare. Here, recent progress on the spectroscopic and photodissociation study of C₂ in VUV region in our laboratory will be presented. The C₂ molecule produced by a discharge valve was photoionized using a tunable high-resolution VUV laser source generated by four-wave mixing technique. We identified four new electronic states of C₂ in VUV region [2-4]. Furthermore, a VUV-pump-UV-probe photoionization scheme was employed to measure the rovibrationally resolved lifetimes in the electronic states. The lifetimes are found to strongly depend on the rotational and vibrational quantum levels, for example in the 2³Σ_g⁻ state as shown in Fig. 1 [5], which indicates that the 2³Σ_g⁻ state may mainly undergo predissociation process through couplings with nearby repulsive electronic states. This observation could have important applications in modeling interstellar medium and cometary comae.

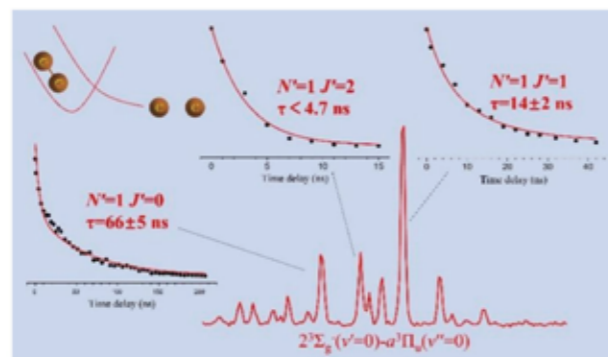


Fig. 1: The rotationally and vibrationally dependent lifetimes measured in the 2³Σ_g⁻ state of C₂ through a VUV-pump-UV-probe photoionization scheme.

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Indicate your choice :

Oral Presentation

Poster Presentation

Rotational Insights into Binding and Aggregation Behaviors of Carbon Dioxide

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The escalating levels of atmospheric carbon dioxide (CO₂), now widely acknowledged as a key driver of global warming and climate change, raise global concern. Carbon capture technologies offer a promising solution in addressing climate change by anthropogenic atmospheric CO₂ levels. This technology involves the selective removal of CO₂ from gas mixtures, followed by desorption, compression, and either sequestration in the underground rock formations (carbon capture and storage, CCS) or utilization in the production of value-added products, including methanol, CO, dimethyl ether, and light olefins (carbon capture and utilization, CCU). The balance between adsorption and desorption is crucial but not always well understood, making judicious selection of capture materials challenging. The formation of complexes and clusters with organic molecules, and their structural and interaction topologies, are critical for these atmospheric processes. High-resolution microwave spectroscopy is the state-of-the-art tool to examine the geometries of weakly bound molecular complexes and clusters in the gas phase. Its high sensitivity to molecular moments of inertia allows the determination of atomic positions from subtle mass distribution variations by even small conformational changes, which manifest as significant shifts in rotational transition patterns. This makes it particularly effective for probing intermolecular NCIs in prototype molecules[1]. Taking advantage of high resolution of rotational spectroscopy, we have systematically analyzed the interaction topologies and structural transitions from dimers [2] to oligomers in clusters involving small organic molecules with carbon dioxide. Additionally, we have examined the competitive interactions between water and carbon dioxide in hetero-ternary clusters, shedding light on their complex intermolecular dynamics [3].

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Indicate your choice :

Oral Presentation

Poster Presentation

Passaging And Resonant Impulse Synergy -

Rotational electric resonance by chirp and single-tone excitation of supersonic jets: PARIS

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Supersonic-jet ‘Fourier transform microwave’ (FTMW) spectroscopy is a powerful tool for studying isolated gas-phase molecules by ‘Rotational Electric Resonance’ (RER) while an extremely low rotational temperature near the thermodynamic zero point can be reached. The established coaxial resonator-jet spectrometer (coaxially oriented beam-resonator arrangement, COBRA) provides unrivalled resolution, but suffers from repetitive, time-consuming frequency retuning of an high-Q resonator to acquire survey spectra. The chirp-excitation method, which employs a short but powerful frequency-ramp signal passaging through molecular resonances, can reduce the survey time dramatically, but at the cost of lower resolution and sensitivity. Even sophisticated coaxial implementations (dual excitation-emission propagation - I/Q-modulation passage acquired coherence technique, DEEP-IMPACT) can regain the resolution, but only some of the lost sensitivity, such that many microwave laboratories are using both spectrometers. With both machines needing molecular sources that might be very sophisticated such as LASER-ablation, a vacuum system capable of handling the jet-expansion at appreciable repetition rate as well as high-frequency electronics and computerized control set-ups, this tends not only to be expensive but also requires turn-over time. We developed and implemented an FTMW spectrometer capable of both techniques with an innovative and resource-efficient approach: Using an elegant design, most electronic components will be used in dual-purpose while integrating both jet-expansion setups in a single vacuum chamber. The single-tone- and chirp-excitation jet-axes are arranged perpendicularly in the spherical chamber of a single instrument named PARIS, operated in either mode with instant turn-over. Both, the ‘Deep-intensity range’ (RER D) and the ‘Broad spectral bandwidth’ (RER B) arrangements of PARIS, use a microwave propagation coaxial with the molecular jet-expansion. Currently, PARIS achieves a sensitivity of parts-per-billion (ppb) of OCS diluted in Neon (1%) on the resonator axis and parts-per-million (ppm) on the broadband axis. A resolution (full width at half mean, FWHM, of the amplitude spectrum) of about 2 kHz can be achieved with the RER D as well as the RER B experiments, i.e. capable of resolving the complex hyperfine structures (hfs) arising from two ¹⁴N nuclei of 4-methylpyrimidine already in broadband operation.

Indicate your choice :

Oral Presentation

Poster Presentation

Schrödinger’s Cat and Molecular Spectroscopy: Vibrationally Averaged Structures of linear Molecules

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As in the metaphor of Schrödinger’s cat in a box, the world described by quantum mechanics, Nature, is independent of ours. To know what happens in a box, we must make observations, so the results depend on how and when we make observations.

Molecular spectroscopy resorts to observing the transition energies. We can observe, within experimental error, the same value occurs in Nature. However, the structure of a vibrating molecule is different. We can observe exact transition energy in rotational spectroscopy, but at the instant when we observe, the target molecule is activated to a different state. It means we cannot observe the direction of the geometrical displacement on the same molecule at the closest consecutive time sequence. Hence, what we can observe in spectroscopy is the unsigned value of the geometrical displacement. Conventional spectroscopy has not paid attention to this issue.

We determine the molecular structure for a linear molecule from the effective rotational constants B_{eff} , which is the expansion coefficient in “energy” and exact. However, when we derive the geometry from there, we must remember that what we observed is the unsigned value of displacement from the origin.

Take the bending motion of a linear molecule (a molecule having the potential energy minimum at its linear structure). The bending motion occurs evenly in plus and minus directions; hence, the average structure is linear (for the cat in the box). We observers (outside the box) cannot distinguish the plus and minus signs of bending motion, so a linear molecule is observed as bent.

This means that when we derive the molecular structure from B_{eff} (exact, because B_{eff} is an energy term), we must abandon the idea of plus-minus canceling for the bending angle to give a linear structure.

The vibrationally averaged structure of a linear molecule is linear, as conventional wisdom in molecular spectroscopy predicts (the cat in the box). However, the structure is observed as being bent (for an observer outside the box). Quantum mechanics presents a method to know how it occurs in Nature: an expectation value calculated over the relevant vibrational wavefunction (Axiom).

Hirano, Nagashima, and Per Jensen first proposed in 2008 an assertion that a linear molecule is observed as being bent. Table 1 shows the averaged deviation angle from linearity, $\bar{\rho}$, in the zero-point structure. In Table 1, “Expect. value” means the expectation value calculated over the bending wavefunction, and “From B_0 ” is the value calculated experimental $B_{0,\text{eff}}$ without an *a priori* assumption that a linear molecule should take a linear averaged structure. The agreement between them is excellent. It means that the vibrationally averaged structure is linear (for the cat in the box), but is observed (by us outside the box) as being bent.

Similar arguments can also be done for the stretching motion. Table 2 compares Mg–O distances from different sources. The Mg–O distance to be observed by us outsiders, i.e., the expectation value over the stretching wavefunction, $\langle r \rangle_0$, is longer by 0.0020 Å even at the zero-point state, and the difference becomes larger for the higher stretching vibration states.

We have to switch to the expectation value when we analyze the experimental values. A paradigm shift is required.

Table 1 $\langle \bar{\rho} \rangle_0$ of linear molecules

	$\langle \bar{\rho} \rangle_0$	
	Expect. Value	From B_0
¹ Σ CO ₂	6.7°	8.8°
³ Σ ⁻ FeCO	7.4°	9.5°
² Π NCS	7.8°	7.8°
² Π BrCN ⁺	8°	
³ Φ CoCN	8°	
² Σ ⁺ MgNC		9.1°
² Δ NiCN	9°	
⁶ Δ FeCN	11°	
¹ Σ ⁺ HCO ⁺	11.0°	12.5°
¹ Σ ⁺ DCO ⁺	9.8°	9.8°
¹ Σ ⁺ HCN	12.0°	14.3°
¹ Σ ⁺ DCN	10.7°	11.6°
⁶ Δ FeNC	13°	
¹ Σ _g ⁺ [XeHXe] ⁺	13.4°	
¹ Σ CsOH	17°	
¹ Σ ⁺ C ₃	19.7°	22.5°
² Σ ⁺ MgOH	26.4°	26.8°

Table 2. Mg–O bond distance (in Å) from various sources.

State	r_{Morse}	r_{sp}	$\langle r \rangle_0$	$r_{\text{obs}}^{(1)}$	Difference from $\langle r \rangle_0 / \text{Å}$		
					r_{Morse}	r_{sp}	r_{obs}
Equilibrium	1.7489			1.7482			
$v=0, J=0$	1.7530	1.7529	1.7549	1.7523	-0.0019	-0.0020	-0.0027
$v=1, J=0$		1.7569	1.7670	1.7604		-0.0101	-0.0065
$v=0, J=0$		1.7626	1.7793	1.7687		-0.0167	-0.0106

¹) Kagi, Kawaguchi, *J. Mol. Struct.*, **795**, 179 (2006) (Analyzed as Cat in a box).



Biography: Gao-Lei Hou is a professor at Xi'an Jiaotong University. He obtained his B.S. and Ph.D. degrees from the University of Electronic Science and Technology of China (2009) and the Institute of Chemistry, Chinese Academy of Sciences (2014). From 2014 to 2021, he conducted postdoctoral training with partial teaching duty at Pacific Northwest National Laboratory, ETH Zurich, and KU Leuven. With backgrounds in chemical physics, molecular physics, and quantum chemical computations, he is now working at the interfaces of physics, chemistry, and astronomy, with research interests in laboratory astrophysics and astrochemistry, catalytic energy conversion and transformation, and cluster-based functional materials.

Affiliation: School of Physics, Xi'an Jiaotong University

Title: Infrared Spectroscopy of Fullerene-metal Complexes and Their Potential Cosmic Relevance

Abstract: Unidentified infrared emission (UIE) bands with wavelengths between 3–20 μm are observed in a variety of astrophysical environments, but over 40 years of research efforts still leave the source of these emission bands largely unknown. In this talk, I will present our innovative approach that combines gas-phase synthesis of fullerene-metal complexes and their in-situ characterization by mass spectrometry, infrared action spectroscopy, and theoretical modeling to understand the carriers of UIE bands. We obtained for the first time the high-quality laboratory infrared (6–25 μm) spectra of gas-phase fullerene-metal complexes, and conducted a detailed comparison with observational Spitzer spectra. We propose that fullerene-metal complexes are promising carriers of astronomical infrared bands, opening a new chapter for studying cosmic fullerene species and carbon chemistry in the Universe.

Rotational Spectroscopy of Complexes and Clusters: From Pure Dispersion to Hydrogen Bond Dominated Interactions

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Rotational, microwave spectroscopy is, in combination with electronic structure calculations, a powerful method to characterize weakly bound complexes and clusters. Analyses of the measured spectra and interpretation of the resulting parameters make it possible to derive information about structures, relative energies, and inter- and intra-molecular dynamics.

In this presentation, I will discuss spectroscopic studies of several molecular systems which differ in their intermolecular interaction strengths. These examples range from rare gas clusters, which are held together by pure dispersion interactions, to hydrated aromatics, which contain strong hydrogen bonds.

The results of those cluster studies affect various aspects of physics and chemistry. For example, they are used as highly accurate benchmarks for the evaluation of electronic structure calculations, shed light on the transition between the microscopic, molecular regime and the bulk phase, and provide insights into aggregation, such as solvation or the formation of aerosol particles.

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Poster Presentation

Nonadiabatic Dynamics and Time-Resolved Pump-Probe Spectra

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Short CV:

Zhenggang Lan's academic journey began with a BS from the University of Science and Technology of China, followed by an MS from the Institute of Chemistry, CAS. He then pursued his Ph.D. in Germany at the Technical University of Munich under Prof. Dr. Wolfgang Domcke. Lan continued his postdoctoral research in Germany at the Max-Planck-Institute fuer Kohlenforschung, where he subsequently assumed a research position. In 2011, he was selected for the CAS "Hundred-Talents Program" and served as a researcher at the Qingdao Institute of Bioenergy and Bioprocess Technology, CAS. Since 2018, he has been a professor at South China Normal University. His research primarily focuses on theoretical and computational chemistry, especially photophysical and photochemical processes, employing various theoretical approaches and machine learning to understand light-induced reactions in chemistry, biology, and materials science. He has achieved multiple results both in the development of theoretical simulation methods and in the study of realistic molecular systems, publishing over 110 papers. He has undertaken and participated in many projects, currently leading two national-level projects and participating in one.

Abstract:

Nonadiabatic dynamics widely exist in photophysics, photochemistry and photobiology. We tried to develop theoretical approaches to study the photoinduced nonadiabatic dynamics. As time-resolved spectroscopy is a very important tool to study the ultrafast dynamics, it is necessary to simulate these spectral signals for the understanding of the experimental observations. We combined the doorway-window representation of the nonlinear response theories and ab initio nonadiabatic dynamics to simulate various time-resolved pump-probe spectra, including transient absorption spectra, time-resolved fluorescence spectra and two-dimensional electronic spectra. We also combine the trajectory surface hopping dynamics and the elastic scattering theory to simulate the ultrafast electronic diffraction signals.

Full dimensional intermolecular potential energy surface construction and spectroscopic calculation for van der Waals complexes

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Van der Waals (vdW) complexes play a significant role in the interstellar medium and planetary atmospheres. The formation and collisions of these complexes can impact the spectral data detected by experiments, making it challenging to distinguish the experimental spectral lines. In recent years, theoretical computational methods have made remarkable progress in the spectroscopic calculation of vdW complexes. In particular, the development of electronic structure methods and potential energy surface (PES) fitting methods makes it possible to construct full-dimensional and spectroscopically accurate PESs in the first principle. This provides a solid foundation for studying complex dynamical simulations, particularly the intramolecular-intermolecular couplings.

In our recent research, we introduced the MLRNet model^[1] that can efficiently fit full-dimensional PESs with physically meaningful asymptotic behavior. We employed an uncertainty-driven active learning approach for point sampling^[2]. This approach reduces the number of sampling grids by nearly an order of magnitude with minimal loss of accuracy. We have tested an uncertainty-driven active learning approach developed for neural network models and found that the algorithm is feasible for both the MLRNet and the PIP-NN models. For the H₂O-He system, about 400 points are enough to achieve a RMSE of 0.3 cm⁻¹ of a large test set. We modularized the computational procedure and made it possible to do the automatic PES construction. We showed that the symmetry-adapted basis expansions with spherical harmonic functions and Hermite polynomials are efficient in obtaining highly accurate long-range functions. For the H₂O-He system, a long-range fitting RMSE of 0.0009 cm⁻¹ ($R \geq 8 \text{ \AA}$) can be obtained with only 240 basis functions, which provides a reliable asymptotic behavior for quantum dynamics simulations in low temperatures. We have further developed a full-dimensional spectroscopic calculation program for nonlinear molecules plus atom systems, and investigate the effect of intramolecular vibrations on intermolecular ro-vibrational spectra based on a full-dimensional potential energy surface^[3].

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Indicate your choice :

Oral Presentation

Poster Presentation

Capturing Transient Species in Ionized Liquid Water

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The ionization of liquid water serves as the principal trigger for a myriad of phenomena that are relevant to radiation chemistry and radiation biology. The earliest events that follow the ionization of water, however, remain relatively unknown. Of particular interest are the lifetime of the transient water radical cation ($\text{H}_2\text{O}^{\cdot+}$) and the fate of the electron that is injected into the conduction band of water by ionization. Femtosecond soft X-ray free-electron laser probing at the oxygen K edge tracks the primary proton transfer reaction of ionized liquid water [1]. The experimental results suggest that $\text{H}_2\text{O}^{\cdot+}$ undergoes proton transfer to yield vibrationally excited hydroxyl radicals (OH^{\cdot}) on the timescale of 46 ± 10 fs. Ab initio molecular dynamics simulations reproduce the experimentally observed ~ 50 -fs component and reveal that it originates from solvation dynamics that accompany proton transfer. By employing few-cycle pulses in the visible to near-infrared (500 – 900 nm) and the short-wave infrared (0.9 – 1.7 μm), we have probed the fate of the electron that is initially injected into the conduction band by ionization. The results suggest that the conduction band electron relaxes to the hydrated *s* electron via an intermediate state with a lifetime of 62 ± 10 fs, identified as the elusive *p* excited state [2]. Ab initio quantum dynamics yield similar lifetimes for these states and furthermore reveal vibrational modes that participate in the different stages of electronic relaxation. Recent extension of these studies to the mid-infrared (2.7 – 8.5 μm) reveals the presence of a broadband transient absorption at sub-picosecond time delays. Our results shed light on the elementary ultrafast dynamics that accompany the interaction of ionizing radiation with liquid water.

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Density Functional Theoretical Study of Tris(cyclopentadienyl)lanthanide in Solid Argon Matrices

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The cyclopentadienyl (C_5H_5 : Cp) complexes are the most fundamental organometallics, which have some forms as following: MCp_2 , MCp_3 , MCp_4 (M: center metal). Tris(cyclopentadienyl)lanthanide (LnCp_3) are the first reported organometallics of lanthanide [1]. The crystal structure of LnCp_3 has a polymeric chain structure and, the bonding nature of LnCp_3 in the crystal are different with depending on the kind of central metals. In liquid phase, LnCp_3 forms ligand adducts molecule, and in gas phase, LnCp_3 decomposes with forming cyclopentadiene (C_5H_6 : CpD) because it is air and moisture sensitive, therefore its monomeric structure of LnCp_3 has unknown precisely.

Matrix-isolation is a powerful technique for understanding the structure or reactivity of unstable molecules or intermediates because those species are trapped in an inert solid, such as low-temperature argon. Using this technique, we determined the monomeric structure of ScCp_3 [2] and YbCp_3 [3], respectively. In this study, we obtained the sample of LnCp_3 isolated in solid argon matrices using the home-made crucible for sublimation of LnCp_3 . The structure of matrix-isolated LnCp_3 was investigated by a joint use of IR spectroscopy and DFT calculations. In particular, the difference of the observed wavenumbers in IR spectra of LnCp_3 depending on the kind of center lanthanide atoms will be discussed.

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Title: Vibrational perturbation theory for energy splitting in symmetric double well potentials

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Weizmann Institute of Science

Abstract: A central advantage of vibrational perturbation theory is that it is readily amenable to first principles quantum chemistry computations and provides a direct route to compare theory with experiment without ad-hoc assumptions. However, the standard second order vibrational perturbation theory for tunneling is not very good especially in the deep tunneling region, due to the fact that it is based on an expansion around the barrier top. In this talk we describe recent developments in vibrational perturbation theory, which enable it to merge with instanton-based theory. The result is a theory which can provide reliable double well splitting for ground and excited state energies in the well. Both second order and fourth order results will be presented.

Broadband Microwave Spectroscopy of Asymmetric Top Molecules Solvated with Helium Atoms

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Although rovibrational spectra of asymmetric top molecules embedded in helium nanodroplets are routinely acquired using IR techniques, MW spectroscopy of small molecule-(⁴He)_N clusters has been limited to linear molecules. In fact, few theorists have studied the size-resolved rotational dynamics of asymmetric tops embedded in Bosonic solvents, with only a few studies currently available [1-2]. The potential experimental complications are foreboding: Large partition functions suppress signal intensity; the added degrees of rotational freedom increase potential rovibrational perturbations, and the lack of theoretical predictions make searches difficult. This latter complication is especially an issue for narrow-band Balle-Flygare cavity experiments that were used in many of the early microwave studies.

Thankfully, the broadband nature and sensitivity of chirped-pulse Fourier transform microwave spectrometers circumvents some of these limitations. Here, we show results using a 2.0-6.0 GHz CP-FTMW spectrometer to identify ⁴He clusters doped with (slightly) asymmetric tops. We use two nitrogen-containing molecules, pyridine and benzonitrile, as our chromophores, because of their large dipole moments and the resulting nuclear quadrupole hyperfine splittings which can be used as spectroscopic fingerprint. By use of pressure dependence, we can systematically identify rotational transitions associated with these clusters. In the case of pyridine, we can identify rotational transitions for clusters containing as many as 20 ⁴He atoms. We will discuss intriguing spectroscopic results for these systems, which reveal surprising and undescribed phenomena and dynamics.

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Probing the ¹(TT) State of TIPS-Pentacene by Heterodyne-detected Sum Frequency Generation Electronic Spectroscopy

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Pentacene and its derivatives are widely studied and utilized as active materials for solar cells due to their optical properties of singlet fission. Singlet fission is a photophysical process where a high-energy photon generates two low-energy triplet excitons, potentially allowing solar cells to break the S-Q limit. The ¹(TT) state in singlet fission is considered a coherent state, which is crucial for the efficient generation of triplet excitons from singlet excitons. However, the characteristic spectral features of ¹(TT) state are mostly inferred from dynamic processes, making it challenging to obtain direct spectral features and precise energy level positions of the ¹(TT) state. In this report, we have developed double resonance electronic SFG spectroscopy by integrating polarization combination and phase-resolved heterodyne detection. This approach enabled us to directly acquire the electronic spectrum of the ¹(TT) state in TIPS-pentacene thin film on quartz, providing significant insights into the singlet fission process.

INTERMEDIATES IN SINGLET FISSION AND TRIPLET FUSION

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Abstract: The photophysical processes of singlet fission and triplet fusion have numerous emerging applications. They respectively involve the separation of a photo-generated singlet exciton into two dark triplet excitons and the fusion of two dark triplet excitons into an emissive singlet exciton. The role of the excimer state and the nature of the triplet-pair state in these processes have been a matter of contention. We have carefully analysed the room temperature time-resolved emission of a neat liquid singlet fission chromophore. It exhibits three spectral components: two that correspond to the bright singlet and excimer states, and a third component that becomes more prominent during triplet fusion. This spectrum is enhanced by magnetic fields, confirming its origins in the recombination of weakly-coupled triplet pairs. It is tentatively attributed to strongly coupled triplet pair state. These observations unite the view that there is an emissive intermediate in singlet fission and triplet fusion, distinct from the broad, unstructured excimer emission.

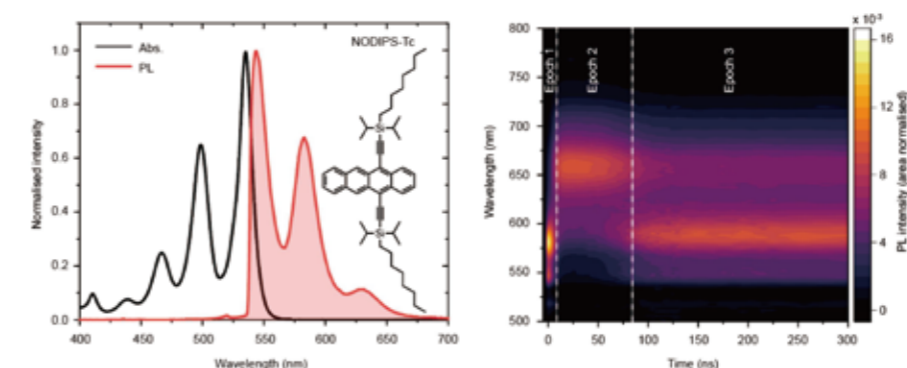


FIG 1: A molecular traffic light! Normalised time-resolved emission of NODIPS-tetracene.¹

¹ J. Feng, et al., *Magnetic fields reveal signatures of triplet-pair multiexciton photoluminescence in singlet fission*, Nature Chemistry. In press (2024)

WaterFEL: Advancing Molecular Spectroscopy and Diffraction with Cutting-Edge Electron-Based Methods

Germán Sciaini*

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Observing atomic motions during chemical reactions and phase transformations has long been a coveted goal in scientific research. The advent of ultrashort electron and X-ray pulses for ultrafast diffraction has transformed this aspiration into reality [1, 2].

Our laboratory's primary research focus is on investigating dynamical phenomena in solid-state materials [3] and solution phases [4, 5], utilizing a range of ultrafast techniques. These include femtosecond broadband transient absorption spectroscopy, time-resolved electron diffraction [6], and the development of advanced electron imaging methods [7]. We emphasize the observation of delicate biological specimens under near-native environmental conditions.

In this talk, I will discuss the technological advancements that have enabled this level of precision, review the current forefront of the field, and outline our plans to establish an integrated infrared free-electron laser (IR-FEL) [8] and ultrafast electron diffraction (UED) [1, 2] facility at the University of Waterloo, known as WaterFEL. This facility will support advanced spectroscopic and structural studies of gaseous, liquid, and solid samples.

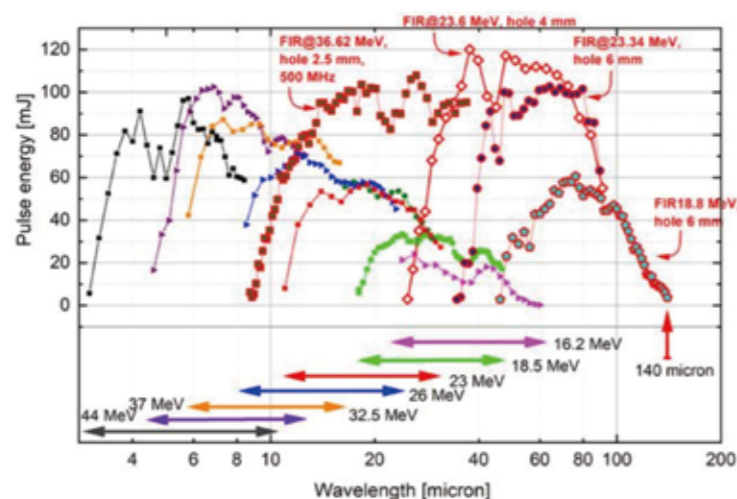


Fig. 1: Power spectrum of Water-FEL based on the Fritz Haber Institute IR-FEL.

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Infrared Spectroscopy of the NO₃ Radical

Jian Tang

Okayama University

High resolution rotation-vibration spectrum of the NO₃ radical in the electronic ground state has been studied extensively and the vibrational assignment in dispute has been understood by the detailed rovibronic analysis which is consistent with the high-level theoretical calculations and the other experimental evidences.

Physicochemical behavior of radicals adsorbed on ice: Application of REMPI method for in situ detection

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Molecular clouds in space are the birthplace of stars and planets. More than 150 chemical species have been identified regardless of extreme physical conditions in molecular clouds: i.e., temperature as low as 10 K, low gas density of 10^3 – 10^5 cm⁻³ (mostly H₂), and very low photon flux. It has been considered that chemical reactions occurring on the surface of low temperature cosmic icy dust play important roles in the formation of these species. To better understand the physicochemical processes occurring on the surface, we should know the elementary processes such as adsorption, surface diffusion, chemical reaction, and desorption. Due to very low temperatures, radical-radical reaction as well as H-atom tunneling reaction plays crucial roles. Because of difficulties, experimental studies on physicochemical behavior of free radicals (including atoms) based on direct detection have been quite limited. An experimental method is required to achieve high sensitivity, surface and species selectivity, and the capability of in situ (quantitative) observation. Recently, we developed a novel method, which fulfills the above requirements, by combining photostimulated desorption and resonance-enhanced multiphoton ionization (PSD-REMPI) to sensitively detect trace amounts of surface adsorbates [1,2]. In this talk, I will introduce the PSD-REMPI method and its applications to the behavior of carbon atoms on low-temperature water ice [3,4].

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Surface for spectroscopy: selection rules and question on the vibrational normal mode

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Second-order nonlinear spectroscopic techniques, such as the sum-frequency generation vibrational spectroscopy (SFG-VS), have been used to study molecular interfaces in the past three and more decades. Interfacial molecules are with specific orientational structures, and their SFG vibrational spectra not only contain the Raman and Infrared (IR) spectroscopic information of the interfacial molecules, but also have strong polarization dependence that can be used to determine the symmetry properties of the molecular vibrational transitions. Thus, an explicit set of spectroscopic polarization selection rules were developed for polarization dependent SFG spectra. Using these selection rules the symmetry properties of each vibrational peak in the SFG vibrational spectra can be elucidated from the observed SFG spectra, independent from the spectral assignments of previous Raman or IR studies, which were often problematic or questionable because of lacking polarization data or of over-congestion of spectra. Based on these selection rules and SFG polarization dependent spectra, misassignments of the vibrational peaks in the Raman and IR spectroscopy based on the bulk phase data can be re-examined and questioned. One of the important examples of such re-examination and questioned problem is the existence of vibrational normal modes in (at least some) simple molecules, which has been the cornerstone in spectral analysis and assignment in vibrational spectroscopy studies.

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Indicate your choice :

Oral Presentation

Poster Presentation

Quantum Phase Synchronization via Exciton-Vibrational Energy Dissipation Sustains Long-lived Coherence in Photosynthetic Antennas

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Abstract

Coherent energy transfer is a highly efficient energy transfer pathway in photosynthesis. Matching of long-lived quantum coherence to the time scale of energy transfer is a prerequisite. In contrast to short-lived electronic coherence, the presence of exciton-vibrational coherence in photosynthetic systems can account for the observed long-lasting quantum coherence. However, uncovering the mechanism of such coherence within a biological environment is challenging because of the presence of noise typically encountered at room temperature. This talk presents conclusive evidence of the existence of long-lasting electronic vibronic coherence in the allophycocyanin trimer, in which pigment pairs behave as excitonic dimers with weak exciton-vibrational coupling. Employing ultrafast two-dimensional electronic spectroscopy, our study demonstrates an extension of the exciton-vibrational coherence time within the trimer compared with the isolated pigments. The prolonged quantum coherences were identified as arising from the quantum phase synchronization of the resonant vibrational collective modes for the pigment pair. The anti-symmetric resonant collective modes undergo fast energy dissipation when coupled to the delocalized electronic states of fast dephasing, while the decoupled symmetric resonant collective modes survive. The nuclear motion of the symmetric resonant collective modes leads to the correlated energy fluctuation of the excitonic energy levels on the two individual pigment molecules in the dimer, resulting in significantly lowered energy dissipation and supporting long-lasting quantum coherences. The presence of the quantum phase synchronization was confirmed by two experimental indicators consistent with the expectation, i.e., about half reduction in the vibrational intensities of the resonant modes and their almost zero intensities in dynamical Stokes shift spectrum. This paper provides direct evidence revealing how biological systems effectively employ a quantum synchronization strategy to uphold persistent coherences, and our findings pave the way for protecting coherences against the noisy environment in quantum biology.

Reference

Zhu R. et al., *Nature Communications*, 2024, 15:3171

Probing the Effect of Solvation of Excited State Molecules

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The conventional ultrafast pump-probe spectroscopy has primarily focused on examining the formation and decay of the excited state intermediates, but it is very difficult to detect those intermediates while the formation is slow and dissipation is much fast, because of the limited concentration during the intrinsic photocycle. To address this issue, a multi-pulse ultrafast pump-dump-probe spectroscopy was employed to generate and probe the short-lived ground state intermediates (GSIs) in an electronic push-pull pyrene derivative (**EPP**). This particular derivative undergoes planarized intramolecular charge transfer (PICT) in the excited state upon initial femtosecond pulse excitation. After applying the dump pulse once the PICT was formed, the blue shifted transient absorption GSIs with the ground state dynamics of the structure recovery was directly observed. It is found that GSIs undergo slower reorganization than the PICT formation in the excited state of **EPP** due to solvation effect with different dipole moments of ground states and excited states. These findings provide a comprehensive understanding of the full photocycle dynamics of both the ground and excited states, shedding light on the presence of hidden ground state behaviors.

Besides, we also present the direct observation of excited-state charge redistribution (delocalization/localization). The intramolecular charge delocalization/localization character of a newly synthesized acceptor-donor-acceptor molecule (ADA) has been intensively investigated by femtosecond stimulated Raman scattering (FSRS) together with femtosecond transient absorption (fs-TA) spectroscopy. By tracking the excited state Raman spectra of the specific alkynyl ($-C\equiv C-$) bonds at each branch of ADA, we found that the nature of the relaxed S1 state is strongly governed by solvent polarity: symmetric delocalized intramolecular charge transfer (ICT) characters occurred in apolar solvent, whereas the asymmetric localized ICT characters appeared in polar solvent because of solvation. The solvation dynamics of ADA extracted from fs-TA is consistent with the time constants obtained by FSRS, but the FSRS clearly tracks the excited state intramolecular charge transfer delocalization/localization.

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Multidimensional Widefield Infrared-Encoded Spontaneous Emission (MD-WISE) Microscopy:

Distinguishing Chromophores by Ultrashort Infrared Pulses

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Photoluminescence (PL) imaging has broad application in visualizing biological activities, detecting chemical species, and characterizing materials. Though the spontaneous emission of PL signals can be detected with high sensitivity, it lacks the information on the identity and environment of chromophores. The broad PL bands in the visible wavelength region also limits the total number of simultaneously monitored chemical species. To solve such problems, nonlinear optical microscopies using molecular chromophores have been demonstrated to encode additional information into PL signals. However, such microscopies often operate under the tightly focused confocal configuration due to the high intensity required for nonlinear optical interactions. Herein, we demonstrate a multiplexed widefield imaging method, Multi-Dimensional Widefield Infrared-encoding Spontaneous Emission (MD-WISE) microscopy [1]. Using a pair of femtosecond mid-infrared and visible excitation pulses, MD-WISE can distinguish chromophores, including molecules and quantum dots, that possess nearly identical emission spectra using multiplexed conditions in a three-dimensional space. The space is defined by three independent variables: the temporal delay between the infrared and the visible pulses, and the optical frequencies of the two pulses. The PL emissions from molecules with various functional groups can be distinguished by tuning the infrared pulse to specific vibrational frequencies of functional groups. Quantum dots and molecules can be distinguished in PL images by varying solely the temporal delay. By demonstrating the capacity of registering multi-dimensional information into widefield PL images, MD-WISE microscopy has the potential of expanding the number of species and processes that can be simultaneously tracked in high-speed chemical imaging applications.

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Indicate your choice :

Oral Presentation

Poster Presentation

The Role of Electronic Structure and Solvent Models in Anharmonic Simulation of Chiral Vibrational Spectra

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With the advances in the instruments for chiral vibrational spectra measurement, recorded spectra can now display an unprecedented level of details, including well-resolved non-fundamental bands.[1] The interpretation of these high-definition spectra pushes simulation going beyond the harmonic level. However, methods able to account for the anharmonicity tend to have a huge overall computational cost, that makes them impractical for most systems of experimental interest. Among all the anharmonic methods, the second-order vibrational perturbation theory (VPT2) represents an interesting choice. It can indeed provide accurate results with at a sustainable cost. However, this efficiency comes at the expense of some weaknesses, that are particularly heightened with the simulation of chiral vibrational spectra. One possible consequence is a wrong sign of prediction. Over the last decade, significant work has been dedicated to overcoming the problem of resonances, known to be the Achilles's heal of VPT2. Thanks to the design of a new, rigorous protocol to identify and correct resonances, it has been possible to ascertain that the resonances in intensity are not the only cause of the wrong sign prediction.[2] To explore the root of the wrong sign problem, electronic structure calculation and solvent models have been re-examined again at the anharmonic level. In this presentation, we will use camphor and fenchone as study cases to show how the solvent effects and electronic structure calculation can fundamentally influence the final anharmonic VOA spectra.

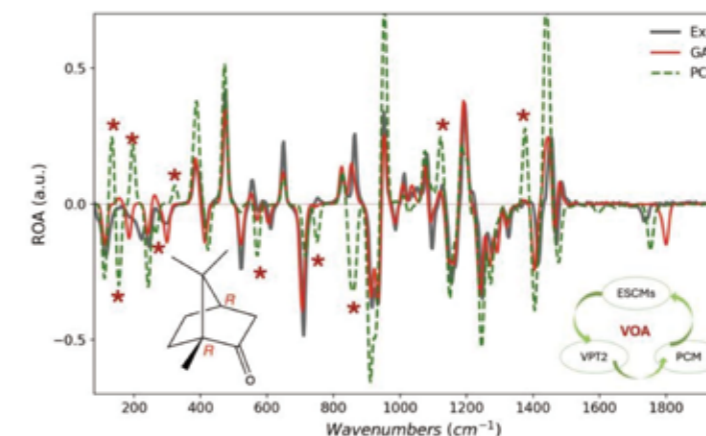


Fig. 1: The abstract may include equations and figures. They should be embedded in the abstract document.

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Indicate your choice :

Oral Presentation

Poster Presentation

Excited-State Dynamics in Organic Photovoltaic Systems under Solar Light Equivalent Excitation

Chunfeng Zhang

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Excited-state dynamics are essential for solar energy conversion devices. Ultrafast spectroscopy, such as transient absorption and terahertz spectroscopy, has been widely applied to monitor the excited-state dynamics that regulate charge generation during the photovoltaic conversion process. Due to limitations in detection sensitivity, the excitation densities used in testing far exceed the operational conditions of actual devices. To overcome these limitations, we have developed a low-noise, high-speed spectroscopic detection scheme that significantly enhances the sensitivity of transient absorption and terahertz spectroscopy, allowing for accurate characterization of the excited-state dynamics of photovoltaic materials under solar light equivalent excitation. We have conducted in-depth studies on the mechanisms of photocharge generation in non-fullerene organic photovoltaic systems and, for the first time, directly observed the terahertz spectroscopic response of charge generation dynamics under solar illumination conditions in these systems. Through these studies, we uncovered a charge generation channel enabled by intra-moiety delocalized excitations, which helps to avoid charge loss at the donor-acceptor interface. Based on these new insights, we further explored the design of high-efficiency planar heterojunction devices.

Femtosecond optics and X-ray lasers study of chloride-pumped rhodopsin

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Light-driven ion pump rhodopsin can convert light energy into membrane potential through active transport of ions. Thousands of light-driven ion-pumping rhodopsins have been discovered that can transport protons, chloride ions, and sodium ions. Here, we study the transport kinetics of chloride-pumped rhodopsin at different salt concentrations. We find that the early dynamics of the retina are strongly dependent on salt concentration.

Nonlinear Spectroscopic Investigation of Supramolecular Chiral Self-Assembly and Dynamics at Interfaces

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The supramolecular chiral assembly at interfaces is crucial for understanding life phenomena and developing new materials. Second-order nonlinear optical methods, with their interface selectivity and sensitivity, are chirality-sensitive techniques and powerful tools for in situ and online studies of supramolecular chiral assembly at interfaces. We utilized chiral high-resolution sum-frequency vibrational spectroscopy, molecular dynamics simulations, AFM, and Brewster angle microscopy to investigate the chiral centers of amphiphilic molecules L-/D-Gan. We found that chirality is formed through weak non-covalent intermolecular interactions, resembling antiparallel β -sheets, and further stacking into macroscopic lamellar structures approximately 900 molecules long and 30 molecules wide (Figure 1 left) [1]. Furthermore, we studied the self-assembly dynamics and mechanisms of achiral TPPS molecules induced by chiral molecules L/D-G12 at the interface. We discovered that the assembly rate increases with the concentration of subphase TPPS and the interfacial film pressure (Figure 1 right) [2]. Further research revealed that subtle changes in molecular structure, such as variations in carbon-carbon bonds and pyridine ring isomerism, can significantly alter supramolecular chiral structures at the molecular level. This study, through in situ observation, elucidates the dynamic process and molecular mechanism of interfacial supramolecular chiral assembly. By linking microscopic intermolecular interactions with macroscopic morphologies, we provides a robust method for quantitatively analyzing supramolecular chiral assembly, linking molecular interactions to macroscopic outcomes, and paving the way for innovative material and drug development.

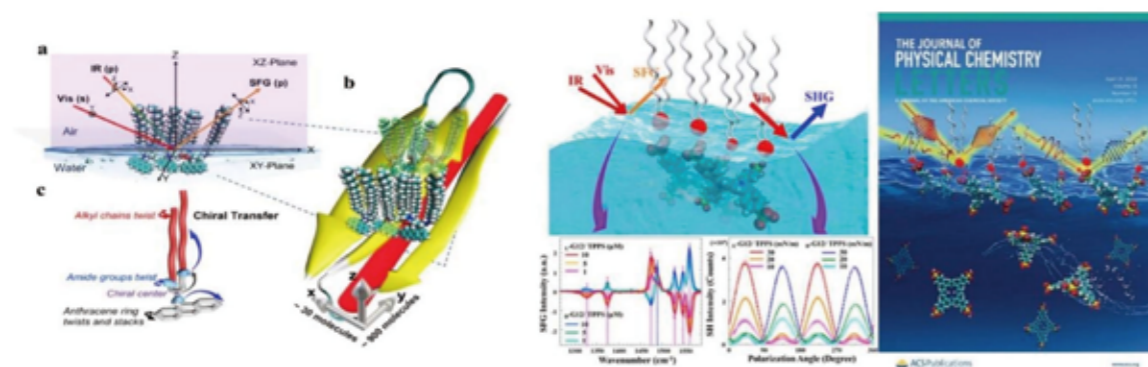


Fig. 1: Interfacial supramolecular self-assembly and its dynamics at molecular mechanism

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Oral Presentation

Poster Presentation

Optical Coherent Control of Molecular Reactions in Chemistry and Biology

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Abstract

Optical control of dynamic processes has been challenging yet has been demonstrated in several chemical and biological systems. The control of a reaction passing the widely present conical intersection has not been realized. Here, we can modulate the phase of the excitation pulse to achieve control of an important chemical process, the dynamics of β -carotene to access the conical intersection (CI). We then report for the first time on the optical control of electron transfer (ET) processes in a protein flavodoxin. Such successful demonstration of optical coherent controlled CI and ET in the chemical and biological systems is significant to opening a new direction, especially to control a variety of ET processes in chemical and biological systems.

Heavy-Atom Tunneling Reactions in Cryogenic Matrices

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Quantum mechanical tunneling allows chemical reactions to occur at energies below the reaction barrier due to the wave nature of particles. Initially recognized for its role in reactions involving light atoms like hydrogen, recent research has broadened this understanding to include heavy-atom tunneling phenomena in second-row elements such as carbon and nitrogen. Here, we present spectroscopic observations and kinetic measurements of heavy-atom tunneling reactions conducted in cryogenic matrices. These reactions encompass diverse processes such as breaking peroxide O-O bonds, ring-closure reactions of ozonides, and cis-trans isomerization reactions. These tunneling processes occur through narrow or low-energy barriers and predominantly involve the tunneling of carbon and oxygen atoms, often leading to significant displacements of two or more heavy atoms.

Towards Understanding the Mechanism of the Ultrafast Dynamics of Water Hydrogen Bonding Network In Bulk and Interfaces

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Hierarchical water motions on material surfaces in different conditions (temperature, hydration extent, pressure, etc.), as well as the coupling of this motion with the substrate/solute dynamics is a complex, long lasting, interdisciplinary research topic. We studied, theoretically, the molecular mechanisms of coupling between the picosecond dynamical onset of substrates and their surface water in the subzero temperatures. By combining with neutron experiments, we explored the dynamics of water and the underlying substrates independently below 0 °C across a broad range of materials. Surprisingly, whereas the function-related harmonic-to-anharmonic dynamical transitions in the materials exhibit diverse activation temperatures, the surface water presents a universal transition at a common temperature. Further simulations revealed that the universal transition of water results from an intrinsic surface-independent relaxation: switching of hydrogen bonds between neighboring water molecules with a common energy barrier ~ 30 kJ/mol. The iso-configurational ensemble analysis was applied to further study water motion at different local substrate environments, which connected the universal process observed to the water rattling motion within their confining cages, instead of the translational motion of water escaping the local cages. The reaction flow analysis revealed the correlation and causality among the water-water, water-protein hydrogen bond switching and protein surface atom rattling dynamics, which provides a picture about how the motion flows from hydration water into the substrate. The aforementioned energy barrier is passed on to the underlying substrates and drives the temperature dependence of the material-specific flexibility, crucial for the function of the materials below the freezing temperature.

Pure rotational and rovibrational spectroscopy of cyclopropylamine in the far-infrared region: Probing the conformational isomerism

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The pure rotational and vibrational spectra of the ν_{27} -NH₂ torsion of cyclopropylamine (CPA) in the far-infrared region were measured with a high resolution FTIR coupled to synchrotron. The dense and complex spectra arise from the existence of both *trans* and *gauche* conformers. The analysis of the pure rotational spectra between 34 and 64 cm⁻¹ enabled accurate determination of centrifugal distortion and rotational constants of the ground and first two torsional excited states of *trans*-CPA. The study also identified and accurately assigned the fundamental, hot bands and even weak overtones in the 200-550 cm⁻¹ range. A global analysis of over 19000 transitions yielded an accurate determination of the energy levels of the torsional polyads up to $\nu_T = 3$. The torsional levels and their rotational constants were in agreement with theoretical results from quasiadiabatic channel reaction path Hamiltonian (RPH) calculations, highlighting the need for molecular-specific theoretical treatments for large amplitude motions. Additionally, tunnelling components of the torsional fundamental of the *gauche* conformer were assigned based on RPH results and symmetry considerations, which differ from previous experimental and theoretical work.

High resolution infrared spectra of formic acid dimer and trimer

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Formic acid (HCOOH) is the simplest carboxylic acid and can form hydrogen bonds easily with other molecules, including itself. High-resolution infrared absorption spectra of formic acid dimer (FAD) and trimer (FAT) in selected spectral range between 900 and 1800 cm⁻¹ have been measured in a supersonic jet of HCOOH/Ar mixtures with quantum cascade lasers or lead-salt diode lasers. Besides the C-H in-plane-bending fundamental and the C-O stretch Fermi triads [1], vibration-rotation-tunneling spectra of several new fundamentals and combination bands of FAD have been analyzed. In our previous study [2], two C-O stretch fundamentals of FAT (ν_{16} @ 1246.3 cm⁻¹ and ν_{18} @ 1172.3 cm⁻¹) were found to have significantly different line-widths, 0.22 cm⁻¹ versus 0.0025 cm⁻¹, which was interpreted in terms of intramolecular vibrational redistribution (IVR) mechanisms. A newly observed O-H in-plane-bending fundamental of FAT (ν_{11} @ 1407 cm⁻¹) is found to have a line-width of only about 0.0010 cm⁻¹. The mode-specific line-broadening mechanism for FAT is still an open question.

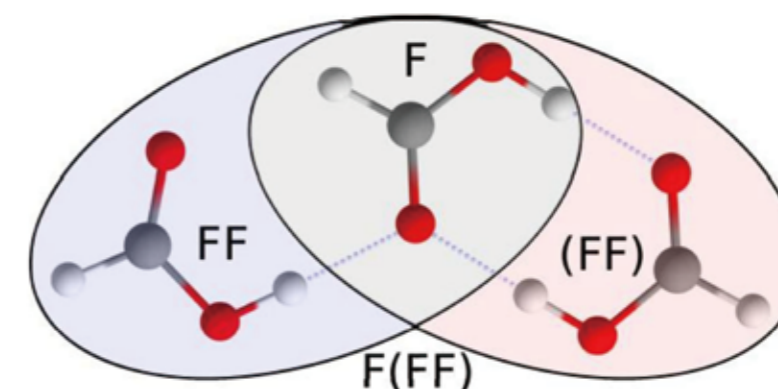


Fig. 1: Connectivities of *trans*-formic acid monomer F, cyclic dimer (FF), polar dimer FF, and trimer F(FF).

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Oral Presentation

Poster Presentation

Rotational Spectroscopic Investigation of the Thiol-Benzofuran Complexes: the Synergistic Role of S–H··· π , S–H···O and C–H··· π Interactions

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Despite the significance of noncovalent interactions of sulfur and aromatic rings in biochemistry, an accurate description of the thiol-heteroaromatic interactions is limited. We investigate the complexes of benzofuran with ethanethiol and 2-propanethiol using chirped-pulse Fourier transform microwave spectroscopy combined with theoretical calculations to explore the features of the noncovalent thiol-heteroaromatic interactions. The experiments revealed that the most stable conformations of both complexes involve the superposition of the thiol molecule over the benzofuran ring face. In the observed structures, the S–H of ethanethiol points to the π -electron of the furan ring assisting the formation of S–H··· π hydrogen bonding interaction while 2-propanethiol forms a S–H···O hydrogen bonding interaction with benzofuran. C–H··· π hydrogen bonding interactions play a synergistic role of stabilization. London dispersion is the main stabilizing term when S–H··· π is the leading interaction and the electrostatic is dominant when S–H···O hydrogen bonding interaction is preferred.

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Poster Presentation

Spectroscopic identification of two Be₂-benzene species featuring Be-Be single bond and pseudo-triple bond

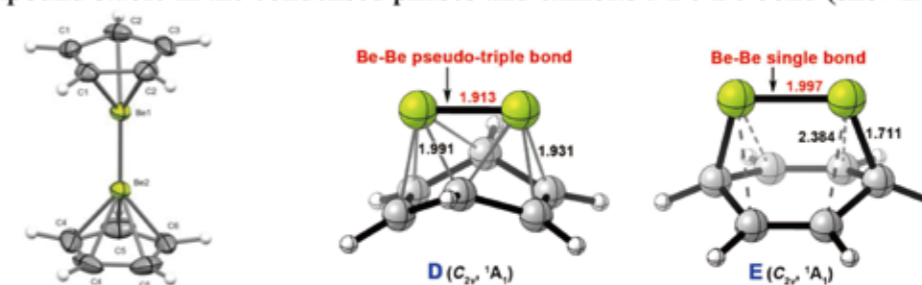
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The formation and characterization of multiple bonds between two beryllium atoms have been the subject of extensive research due to their fundamental importance in understanding chemical bonding and reactivity. However, experimental research on beryllium chemistry has been limited and hindered by the extreme toxicity of beryllium. Additionally, compounds exhibiting Be-Be multiple bonds are highly reactive, unstable, and sensitive to moisture and air, requiring careful handling and storage. Recently, a landmark study by Josef T. Boronski, Simon Aldridge and colleagues reported the synthesis of the complex diberyllocene, CpBeBeCp (Cp, cyclopentadienyl anion) which is an organometallic compound stable in the condensed phases and exhibits a Be-Be bond (shown in **scheme 1**).



J. T. Boronski et al.,^[1]

This Work

Scheme 1. Molecular Structures of CpBeBeCp and Be₂-Benzene compounds

In this study, we successfully synthesized and characterized two Be₂-Benzene species (marked **D**, **E**) in solid neon. These compounds have been identified by infrared spectroscopy with D and ¹³C isotopic substitutions benzene reagents as well as quantum chemical calculations. The Be₂-Benzene complex (**D**) exhibits a unique half sandwich structure with an unusually short Be-Be distance (1.913 Å), which is even shorter than the NHC-supported Be-Be double bond (1.945 Å). Bonding analysis indicates that this structure includes a classical 2c-2e Be-Be σ bond, an 8c-2e σ bond and an 8c-2e π bond in the Be₂C₆ moiety. These results indicated that the Be-Be bond in species **D** can be described as a pseudo-triple bond. The 7,8-diberyllium-bicyclo[2.2.2]-2,5-hexadiene (**E**) is formed at the cost of species **D** under UV light irradiation, which is confirmed to have a Be-Be single bond Be-Be distance of 1.997 Å by high level of quantum-chemical calculations.

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Oral Presentation

Poster Presentation

Analyzing Multi-channel Shape Resonances in Cold Collisions through Wavefunctions

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Rotational transitions in cold (~ 1 K) molecular collisions are often related to single partial-wave (L) shape resonances. These resonances are sometimes attributed to a quasi-bound state supported by an isotropic effective potential for entrance channel [1]. However, their strong dependence on initial alignment of colliding partners implies non-negligible multi-channel coupling due to the anisotropy of interaction potential [2]. Hence, quantization in a multi-dimensional space is needed for a thorough understanding of these resonances. In this work, we analyzed four low-lying shape resonances in rotationally inelastic collisions $para\text{-H}_2$ ($v_1 = 1, j_1 = 2$) + HF ($v_2 = 0, j_2 = 0$) \rightarrow $para\text{-H}_2$ ($v'_1 = 1, j'_1 = 0$) + HF ($v'_2 = 0, j'_2$). Full-dimensional quasi-bound wave functions were obtained for them from stabilization method and utilized in a new model to illustrate the selection rules on initial alignment of molecules.

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Adsorption Configurations and Interaction Behaviors of CO and CO₂ on CoO(001) Surfaces Probed by UHV-PR-FTIRs

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Cobalt oxide nanomaterials show high activity in a few catalytic reactions than noble metals. However, their physical and chemical properties have not yet been studied to date at a molecular level for surfaces of a well-ordered CoO catalyst. Considering that CO is one of the main pollutants in the atmosphere and CO₂ is the main component of greenhouse gases [1,2], in this work adsorption configurations and interaction behaviors of CO and CO₂ as probing molecules on the well-ordered CoO(001) surfaces were in situ explored thereby under ultra-high vacuum (UHV) conditions by the polarization-resolved Fourier transform infrared spectroscopy (PR-FTIRs).

Properties of the single crystal CoO(001) film were characterized by XRD, LEED, and AES,

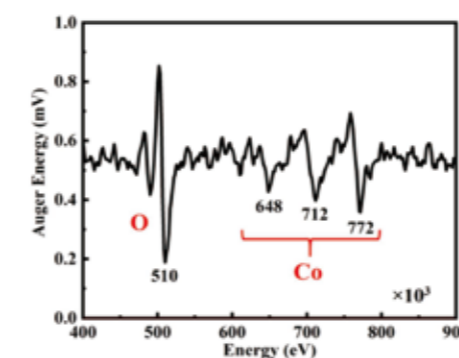


Fig. 1: Pattern of the single crystal CoO(001) film characterized by Auger electron spectrometer (AES). One peak of O at 510 eV and three peaks of Co at 648, 712, and 772 eV can be clearly seen, while no peaks for other elements are seen.

as shown in Fig. 1 for the AES, indicating that the prepared CoO(001) surfaces are clean and well-ordered. The UHV-PR-FTIRs results at 100 K show that CO adsorbs at top sites of the terraces in a nearly vertical manner, the C atom bonds to surface Co²⁺ ions on CoO(001) facets, and the absorption peak of CO continuously red-shifts from 2135 to 2127 cm⁻¹ in exposure range of CO from 0.02 to 0.15 L. Although the O₂ usually adsorbs hardly on CoO(001) surfaces at low temperatures, it adsorbs on the CO-precovered CoO(001) surfaces by reacting with CO to form a complex of CO-O₂ and blue-shifts to 2152 cm⁻¹ via transferring electrons from CO to Co²⁺. Two absorption peaks at 2326 and 2303 cm⁻¹ with close adsorption energies are detected for the physisorbed CO₂ on CoO(001) surfaces. Our current results provide experimental evidences for understanding catalytic reaction

mechanisms of CO and CO₂ on cobalt-oxide catalysis and designing stable cobalt-oxide-based nanomaterials and heterogeneous catalysts.

Acknowledgments: This work was partly financially supported by the National Natural Science Foundation of China (Grant No. 91536105) and the Shandong Provincial National Science Foundation of China (Grant No. ZR2018MA041).

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Oral Presentation

Poster Presentation

Line intensity measurement of CO and H₂ transitions with 0.1% precision

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The frequency accuracy of molecular line positions in the infrared has been improved to the order of 10^{-12} or even 10^{-13} , but a high-accuracy determination of line intensities remains a persistent challenge. Very limited studies have been reported with uncertainties at the level of one-thousandth. Sub-promille precision in line intensities is of great value in various applications, such as planetary atmospheric analysis, trace gas detection, temperature metrology, and pressure standards. Here we report the simultaneous measurement of both cavity-enhanced absorption spectroscopy and cavity-enhanced dispersion spectroscopy of molecules using the same high-finesse cavity. Transitions in the $v = 3 - 0$ band of carbon monoxide near 1.57 micro and the first overtone Q(1) line of the H₂ near 1.2 micro were measured. Both the absorption and dispersion spectra were fitted separately employing the Hartman-Tran profile (HTP), and the results obtained by the two methods are in excellent agreement. The line intensities were determined with uncertainties of around 0.1%, and the deviations from the theoretical results are within 0.2%. The results indicate promising prospects for SI-traceable, high-precision molecular density measurements based on laser spectroscopy.

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New A²Π -X²Σ⁺ Bands of CaH

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Calcium monohydride (CaH) is among the few molecular species detected in space. Since its discovery in solar spots in 1908, it has been identified in various environments such as cool stars and brown dwarfs, and is particularly abundant in the atmospheres of M-type brown dwarfs. To accurately calculate absorption coefficients for radiative transport and atmospheric models of brown dwarfs, detailed experimental data on CaH's electronic transitions are required. Spectroscopic measurements of CaH's electronic transitions began in the 1920s, with extensive studies of low-lying states (X²Σ⁺, A²Π, B²Σ⁺, C²Σ⁺, D²Σ⁺, E²Π, K²Σ⁺, L²Π) conducted by the 1970s. These studies revealed local interactions between the vibrational levels of the B²Σ⁺ and A²Π states, as well as strong interactions between the D²Σ⁺ and B²Σ⁺ states. Recently, accurate molecular constants for states such as X²Σ⁺ (v=0-4), A²Π (v=0-3), B²Σ⁺ (v=0-2), and E²Π (v=0, 1) have been calculated from experimental data by researchers like Ram and Shayesteh [1][2].

Our laboratory has previously examined and identified transitions between nearly all vibrational levels of the B/B'²Σ⁺ electronic state (v=3-19) and the X²Σ⁺ state (v=0) [3][4]. In doing so, we observed strong interactions between the vibrational levels of the B/B'²Σ⁺ and D²Σ⁺ states, and found that the energy levels were consistent with theoretical predictions by Carlsund-Levin and colleagues [5].

In this study, we continued by measuring the vibrational-rotational spectra of the high vibrational levels of the A²Π state, specifically the A²Π - X²Σ⁺ (10-0, 11-0) transitions. Using a computational program for fitting, we then determined molecular constants such as T₀, B, D, γ, γ_D, A, p, and q for these states.

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Oral Presentation

Poster Presentation

Investigation of Structures, Vibrational Dynamics, Phase Transitions of Energetic Materials using Mid- and Far- Infrared Spectroscopy

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The vibration modes of energetic materials in the mid-to-far infrared range show high sensitivity to external stimuli. Therefore, mid-to-far infrared vibration spectroscopy has become an effective tool for studying structures, vibration dynamics, and phase transitions of these materials. To date, commercial infrared absorption spectrometers are limited by the wavelength response range of light sources, beam splitters, and detectors, and are less used in related studies. Meanwhile, compared with the synchrotron radiation source beamline, the desktop terahertz light source and detection system are more convenient, the optical setup configurations can be quickly adjusted according to experimental requirements (powder, crystal, film, liquid, high temperature, high pressure, etc.). Therefore, we developed the mid-to-far infrared ultra-broadband spectroscopy based on air plasma, and the wide-spectrum infrared absorption spectra of two-dimensional materials, energetic material crystals, and films were successfully obtained [1]. Combined with the Diamond anvil cell (DAC), The mid-to-far infrared spectra of the structural evolution and vibration coupling dynamics under high pressure of energetic materials such as TATB, HMX, and HN [2] were successfully obtained. Using analysis of first-principles calculations, the intermolecular weak interactions, such as hydrogen bonds, van der Waals forces, and steric hindrance, that affect the variation of molecular stacking in the crystal with increasing pressure were revealed. Furthermore, the structural evolution and phase transition processes of TATB, HMX and HN under high pressure were obtained. The changes in vibration dynamics under pressure indicate that pressure enhances multi-phonon coupling and intra-molecular energy transfer.

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Oral Presentation

Poster Presentation

Mechanism and Regulation of Metal Ion-Induced Phase Separation in Peptide Solutions

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The Liquid-liquid phase separation (LLPS) is ubiquitous in living systems, enabling the functional regulation of biomolecules through the establishment of biochemical active zones. Consequently, it holds immense promise for applications in drug delivery, biomimetic materials, and beyond. LLPS involves complex protein interactions across multiple time scales, and the core of research lies in how to effectively select and design biomolecular 'modules' to construct biomimetic materials with specific properties and functions. [1] The crux of research lies in the effective selection and design of biomolecular "modules" aimed at fabricating biomimetic materials with tailored functions and properties. Guided by this principle, we have selected a highly repetitive peptide sequence (GH16) from the natural jaw protein of bloodworm, which shows outstanding phase separation and catalytic activity. This sequence is composed solely of glycine and histidine, and forms coacervate droplets upon chelation with copper ions. To elucidate the copper coordination and catalytic mechanism of the droplets, we employed two-dimensional infrared (2D IR) spectroscopy technology. Through a series of oligopeptides, we established the correspondence between various copper-ion binding sites and IR spectral features, revealing the existence of two distinct binding sites within GH16, each serving distinct functions in the dopamine catalytic process. [2] 2D IR spectroscopy effectively distinguished the characteristic spectral information of copper ions binding to different groups in histidine-containing peptides (Figure 1), with the histidine side chain exhibiting particularly notable features, including a 30 cm⁻¹ frequency shift and intensity increase. Therefore, this method also lays a methodological foundation for further application of transient 2D IR spectroscopy in studying the histidine-copper transport process and pathogenic mechanisms in vivo.

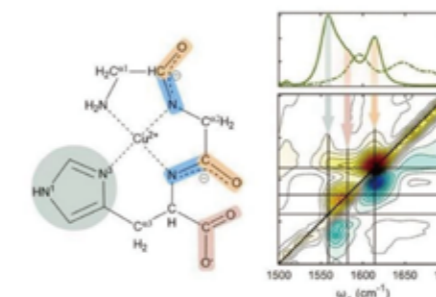


Fig. 1: Structure of Cu^{II}-GGH complex and its FTIR and 2DIR spectra.

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Indicate your choice :

Oral Presentation

Poster Presentation

A molecular dynamics simulation software for polymers

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Abstract

It is a daunting challenge to simulate polymers by molecular dynamics (MD) simulations due to the large size and long relaxation time of polymer chains. Combining coarse-grained models and GPU-accelerated computation, we develop a software for the large-scale MD simulations of polymers. The name of software is PYGAMD (Python GPU-Accelerated Molecular Dynamics Software, <http://pygamd.com/>). It integrates modeling, dynamic simulation engine, property analysis modules with 9 innovative simulation methods. Taking dynamic bond model as an example, we show how MD simulations can reveal the mechanism of enhancing the mechanical properties of polymers by hydrogen or coordinate bond interactions.

- Included by NVIDIA homepage and SklogWiki program library
- Number of published papers with this software >200

Platform for polymer simulation

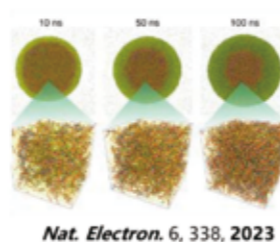
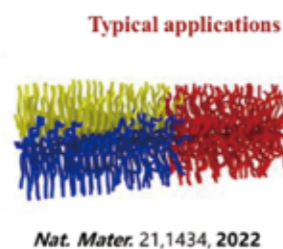
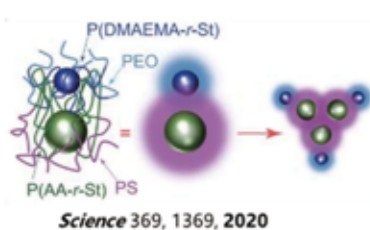
Molecular dynamic program



- GPU-accelerated large-scale molecular simulation toolkit
- Some simulation methods for polymers



- Python GPU-Accelerated Molecular Dynamics
- Self-defined force field (NUMBA)
- On-line installation (commands: pip install pygamd)
- Supporting Python3 and setup installation
- Supporting Hua Wei CPU, NVIDIA GPU and DCU



Reference

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Acknowledgement

This work is supported by the National Natural Science Foundation of China (22133002 and 22273031), the National Key R&D Program of China (2022YFB3707300).

Precision spectral measurement of methane in the

2ν₃ transition band

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Abstract: Methane is a significant component of atmospheric greenhouse gases [1]. To monitor the global distribution and changes in methane concentrations, satellites such as GOAST[2] and MERLIN[3] have been launched into geosynchronous orbit for round-the-clock real-time monitoring. However, due to the high symmetry of the methane molecular structure, its four normal mode frequencies (ν_i) exhibit an approximate relationship: $\nu_1 \approx 2\nu_2 \approx \nu_3 \approx 2\nu_4$, resulting in a very dense methane transition spectrum. Under the Doppler broadening effect, multiple symmetric transitions overlap significantly, making it difficult to accurately obtain their precise frequency values and, subsequently, the spectral line shape parameter with a precision better than 1%. The high precision Doppler- and sub-Doppler absorption spectroscopy [4] at low pressures were applied to the studies of two transition clusters R6 (MERLIN) and R9 (NIM). Not only does it facilitate the determination of frequencies with an accuracy at the several kHz level for 99 transitions, but it also provides a relative intensity precision superior to 1% for the transitions in the R6 and R9 clusters that are stronger than 1×10^{-23} cm/molecule. The findings indicate that the existing database presents certain deficiencies, potentially causing a deviation of up to 10% in the cross-sections utilized for methane remote sensing.

References:

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- [4] L. -G. Tao, A. -W. Liu, et al, *Phys. Rev. Letts.* **120**, 153001(2018)

Indicate your choice :

Oral Presentation

Poster Presentation

An Atomic Force Microscopy and Total Internal Reflection Fluorescence Microscopy Correlated System (AFM-TIRF) for Fluorescence Imaging and Spectroscopy of a Single Particle

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Combining atomic force microscopy (AFM) with other optical microscopic techniques is pivotal in nanoscale investigations, particularly leveraging the surface-sensitive properties of total internal reflection fluorescence microscopy (TIRF). A novel design that integrates AFM with a multi-wavelength TIRF is displayed, providing simultaneous fluorescence imaging and spectral acquisition capabilities [1]. We elaborated the instrument design process and demonstrated the performance and potential applications of the instrument through fluorescence imaging and spectroscopy testing of individual nanoparticles, demonstrating that the instrument is capable of detection weak optical signals while simultaneously manipulating nanoscale objects.

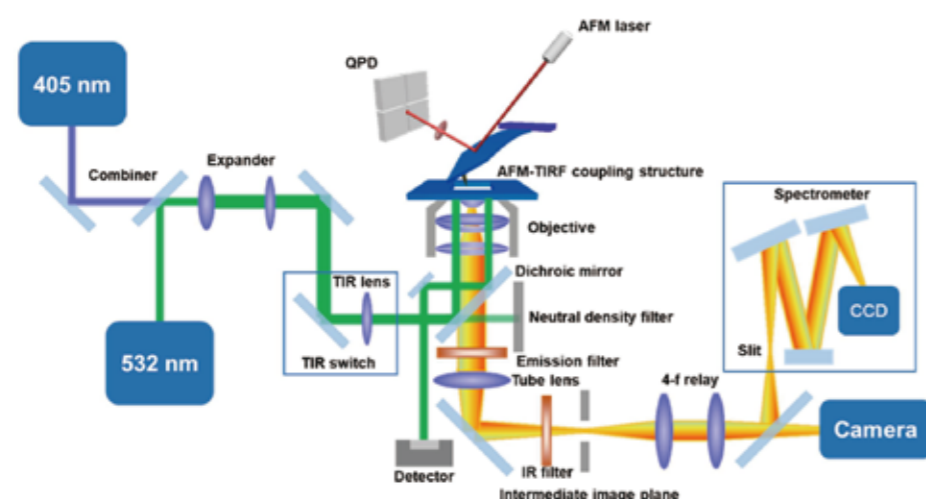


Fig. 1: The abstract may include equations and figures. They should be embedded in the abstract document.

Our AFM-TIRF system possesses excellent imaging and spectral resolution capabilities for fluorescent molecules adsorbed on both individual nanoparticles (20 nm) and the tip of an AFM probe (a radius of curvature of 20 nm). This AFM and TIRF correlated system (AFM-TIRF) emerges as a promising option for single-molecule fluorescence studies, enabling simultaneous manipulation and detection of fluorescence from individual molecules.

References:

[1] Cao X., Wang W., Jiang Y., Feng W., Xu S., Xu W., Zhang W., *Rev. Sci. Instrum.*, **95**,7 (2024).

Oral Presentation

Poster Presentation

Microfluidic Droplet-SERS Platform for Single-Cell Cytokine Analysis via a Cell Surface Bioconjugation Strategy

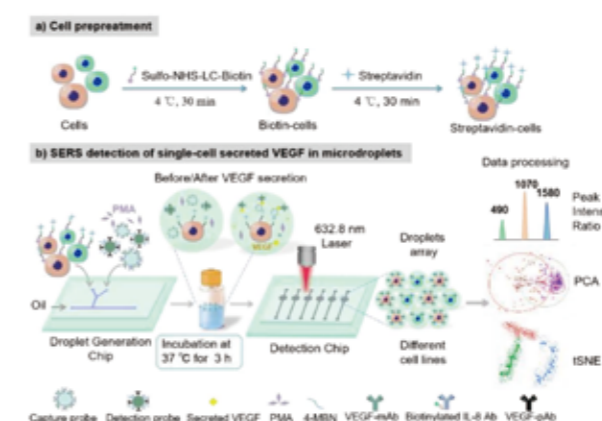
Lili Cong¹, Weiqing Xu¹, Weigang Wang², and Shuping Xu^{1,*}

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To meet the urgent need for fast and sensitive single cells capable of tracking specific secreted cytokines, this study presents a microfluidic-based surface-enhanced Raman scattering (SERS) platform for analyzing cytokines secreted by single cells based on the elaborate bioconjugation of the immuno-sandwich complex on the probed cell surface. (Scheme 1). Firstly, the cell membrane surface was pretreated with biotin (Sulfo-NHS-LC-Biotin) and streptavidin (SA), of which Sulfo-NHS-LC-Biotin enables efficient biotinylation of cell membrane proteins, and is cell membrane impermeable due to its negative charge [1]. Secondly, two types of immunological nanoprobe were introduced. One is the dual-functional capture probe (SiO₂@biotinylated Ab&VEGF mAb) that has the cell membrane protein-targeting nature and the cell-secreted cytokine capturing ability. The other is a SERS detection probe, which is labeled with antibody and Raman reporter molecules, taking charge of the signal output. Then, an immune sandwich structure was constructed on the surface of the cell membrane via VEGF as a bridge, which was used to track the amount of secreted VEGF (Scheme 1). We further combined the microfluidic droplet-SERS technique with chemometrics to identify significant differences in the ability of the three cancer cell lines to exocytose cytokines at the single-cell level, revealing the heterogeneity among individual cells [2]. This platform provides an experimental basis for the use of single-cell cytokine as biomarkers for the early diagnosis of cancer and provides physiological clues for the understanding of single-cell secretion.



Scheme 1. Workflow of the cell pretreatment and the microdroplet-SERS detection of single-cell-secreted VEGF in microdroplets based on the cell surface bioconjugation

References:

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Oral Presentation

Poster Presentation

SERS/UV-vis analyzes the heterogeneous photocatalytic degradation

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Surface-enhanced Raman spectroscopy (SERS) has broad application prospects due to its high sensitivity and accuracy.^[1] TiO₂ can exhibit semiconductor-based charge transfer enhancement mechanism for SERS activity, and the adding of polyoxometalates can modulate the band information of TiO₂, enhancing the synergistic SERS enhancement effect.^[2] In this study, a TiO₂/H₃PW₁₂O₄₀(TiO₂/HPW) composite substrate with surface-enhanced Raman spectroscopy (SERS) activity was prepared to detect malachite green(MG) molecules, which provides a pathway for detecting contaminants.

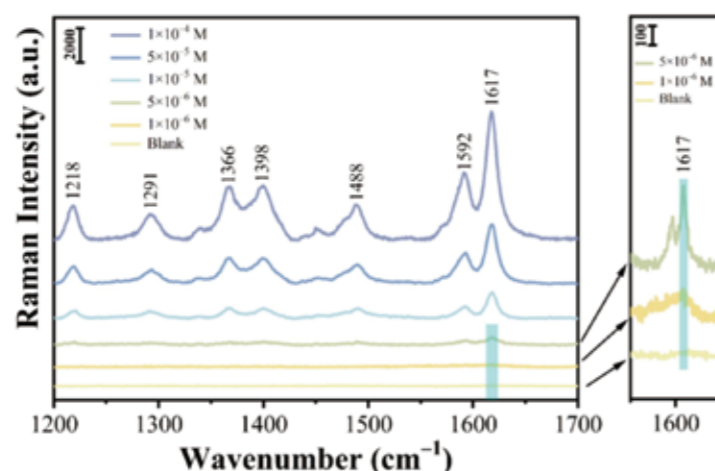


Fig. 1: SERS spectra of MG obtained using TiO₂/HPW NPs as substrates.

References:

- [1] J.J. Chen, M.Y. Li, Y.M. Yang, H. Liu, B. Zhao, Y. Ozaki, W. Song, *J Colloid Interf Sci.* **660**, 669-680(2024).
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Indicate your choice :

Oral Presentation

Poster Presentation

Probing Pre-Reaction Intermediates for Ring-Opening Reactions between Epoxides and Acids

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Abstract: The significance of ring-opening reactions between epoxides and carboxylic acids extends far beyond mere chemical transformations; they serve as cornerstones in the stereoselective synthesis of intricate organic molecules with complex architectures, holding immense potential in pharmaceutical, agrochemical, and materials science domains. [1-2] This study marks the inaugural use of Fourier transform microwave spectroscopy to detect the pre-reaction intermediates in the ring-opening reactions of propylene oxide-formic acid and epichlorohydrin-formic acid within a pulsed jet. Our investigations revealed two distinct intermediate structures in the reaction of propylene oxide, and one in the reaction with epichlorohydrin. The intermediates are predominantly stabilized by hydrogen bonds, which facilitate the protonation of oxygen, a key step in the ring-opening mechanism. These findings describe the crucial role of non-covalent interactions in forming pre-reaction intermediates, summarize their stability and precise molecular structures.

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Indicate your choice :

Oral Presentation

Poster Presentation

Research on Metasurface Regulated Electrochemiluminescence Strategy for Exosome Detection

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Metasurface is an artificial planar electromagnetic material consisting of a large number of periodically arranged sub-wavelength scale structures, drawing a great deal of attention in different fields such as materials science and nanophotonics.¹ Metasurface can flexibly tune electromagnetic wave properties such as amplitude, phase, polarization state and spectrum. Metasurface supports various optical modes including localized surface plasmon resonance (LSPR), surface lattice resonance (SLR), Fano resonance and quasi bound states in the continuum (quasi-BIC). Metasurface possesses optical localization and electromagnetic field enhancement capabilities, making it promising platform in biomedical sensing. Electrochemiluminescence (ECL) can work as the unique background interference-free light source for the metasurface, which is a luminescence phenomenon triggered by electrochemical redox reactions.² ECL combines electrochemistry and chemiluminescence, and has the advantages of low background noise, temporal and spatial control, and fast response, which makes it a competitive analytical detection technique, and can also be used as a unique background interference-free light source for the metasurface. Extracellular vesicles (EVs) are nanosized phospholipid bilayer vesicles secreted by almost all types of cells, which carry a variety of parent-cell-derived biomolecules (e.g., lipids, proteins, mRNA/microRNA, and DNA fragments).³ EVs are a highly regarded cancer marker in liquid biopsies with clinical significance and application value in early diagnosis of tumors and evaluation.

change the original electron cloud density distribution of the nanoparticle lattice and provide excellent optical properties. The plasmon coupling effect and the Purcell effect originate from the tightly packed structure and cavities in the metasurface can produce electromagnetic 'hot spot'. The optical response of the metasurface can be switched by an external magnetic field, which has the advantages of subnanosecond ultrafast response, noncontact, continuous regulation, and environmental friendliness. In the presence of the external magnetic field, Fe₃O₄ nanoparticles can be magnetized and provide a local magnetic field in the metasurface, which further induces the Lorentz force effect to change the moving direction of electrons. ECL signal can be continuously modulated by the magnetoplasmonic metasurface and significantly enhanced at a specific polarization angle. As a result, MECL system ultimately gains highly directional and enhanced ECL signal. Due to the high affinity and specific binding of the mucin 1 aptamer to GC EVs and the catalyzing hairpin self-assembly strategy, MECL sensing system can be used to detect GC-derived EVs in ascites samples. MECL strategy is a universal approach to regulating the optical signal and helps to build a new surface plasmon-coupled emission-based stimulus-response system.

References:

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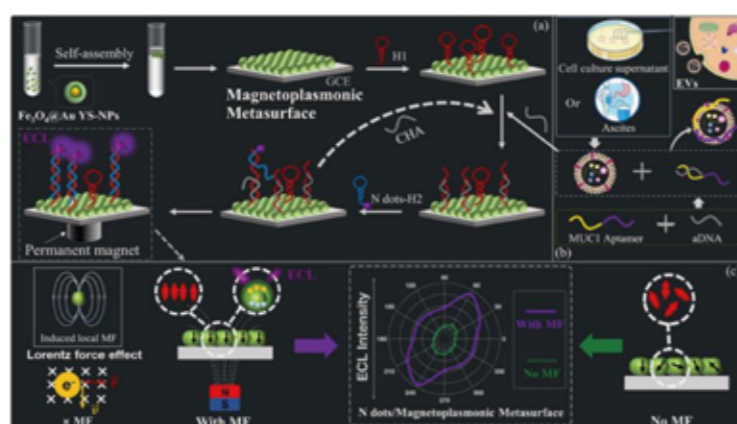


Fig.1 Metasurface-regulated ECL strategy for gastric cancer derived-EVs

This work developed a metasurface-regulated ECL (MECL) strategy for gastric cancer derived-EVs (GC EVs) detection. As shown in Fig. 1, metasurface with yolk-shell Fe₃O₄@Au NPs as meta-atoms was constructed on the glassy carbon electrode by self-assembly. Nitrogen dots were synthesized by microwave-assisted hydrothermal method as ECL emitters. Compared with conventional quantum dots, N dots do not involve the use of heavy metals in their preparation and are easily available, nontoxic, and biocompatible. N dots have higher nitrogen content, and nitrogen atoms with strong electronegativity can

Multienzyme-like aerogel as SERS/colorimetric sensing platform for the fermentation process of tea

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The unique characteristic of tea fermentation is the oxidation of polyphenols, which results in significant variations in the total antioxidant capacity (TAC) of different teas. This study has developed MnO₂@Ag nanoplate aerogels with laccase and oxidase activities, as well as surface-enhanced Raman scattering (SERS) activity. The MnO₂@Ag nanoplate aerogel demonstrated laccase-like activity, efficiently oxidizing catechins to mimic tea fermentation, resulting in the formation of quinone-type oxidation products (oxCC). Furthermore, we utilized MnO₂@Ag aerogels for SERS/colorimetric detection of epigallocatechin gallate (EGCG) down to 1 μM.

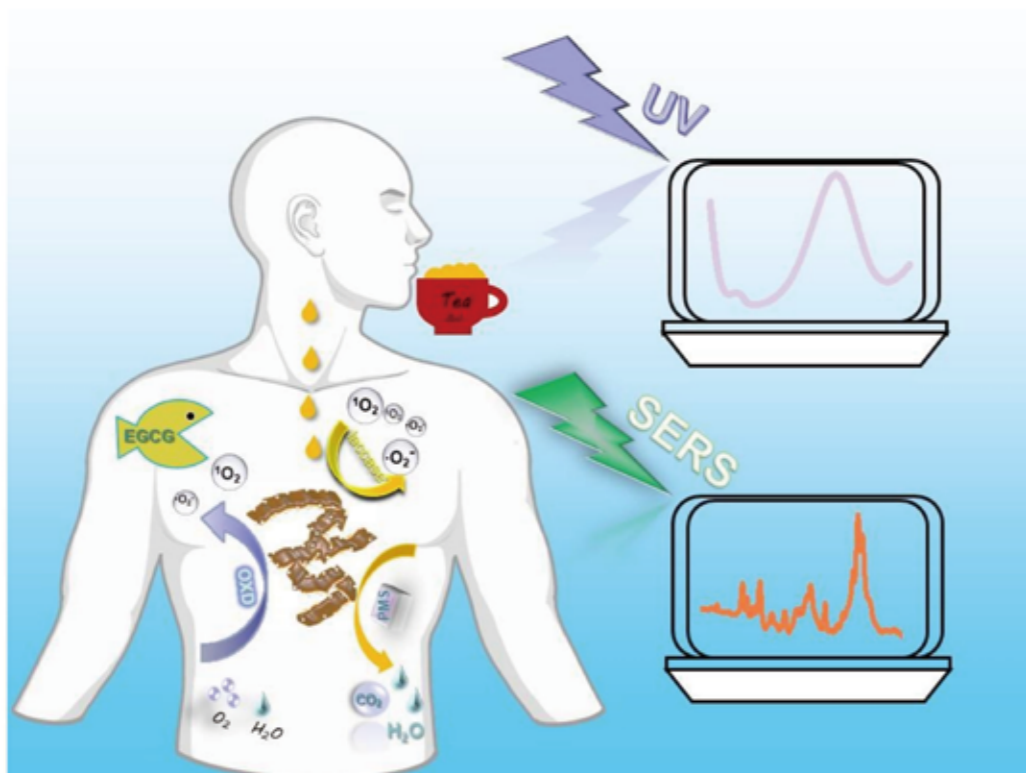


Fig. 1: Schematics of MnO₂@Ag aerogel as SERS/colorimetric sensing platform for tea fermentation process.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

Reveling the ultrafast energy transfer pathways in energetic materials: Time-dependent and quantum state-resolved

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The β-HMX is a widely used representative high-energy crystal, both experimental and theoretical studies have done a lot of on its energy transfer mechanism over the years in order to utilize its explosive properties and to store and transport it more safely. However, the coupling between the vibrational modes and the ultrafast energy transfer process make it challenge for experimental observation. Therefore, in this work, we determine the energy transfer between different vibrational modes and predict the pump-probe spectra. First, the combined distribution function (CDF) based on normal modals coordinates is analyzed to find the strongly coupled vibrational modes, and then the pump-probe spectra are calculated. The complex vibrational spectral regime can be divided into two parts, probe molecules (clusters) and the environment, so obtaining the correct time-dependent transitions, including environmental perturbations, is an important challenge. The local quantum vibration embedding (LQVE) [1] method, which combines molecular quantum vibrations and molecular dynamics with perturbation theory to introduce dynamic environmental effects more comprehensively, has been successfully applied to the simulation of several systems, and has obvious advantages in terms of accuracy and transportability. Classical molecular dynamics is used to describe the dynamical effects in the β-HMX crystal system, considering the quantum effects of atomic nuclei, while quantum mechanics is used to describe the vibrations of the probe molecules. PODVR saves the cost while accomplishing an efficient description of the vibrational state. The structures in each step of the dynamical trajectory are processed with degrees of freedom using our self-developed molecular substitution algorithm, which in turn computes the instantaneous properties of the molecule (e.g., instantaneous vibrational frequency, transition polarization rate, etc.) using the quantum-mechanical approach. Calculating the pump-detection spectra, the coupling of multiple vibrational modes and multiple quantum states can be handled to further accurately describe the energy transfer between important modes.

References:

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Oral Presentation

Poster Presentation

Optical Photothermal Infrared (O-PTIR) Spectroscopic Analysis of Cryptochrome CRY2 protein for its Blue Light-induced Phase Separation Phenomenon

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Phase separation has become a hot topic in life sciences research nowadays[1]. The phenomenon of phase separation embodies problems at multiple important supramolecular levels. However, in many liquid-liquid phase separation (LLPS) systems, droplets cannot be directly extracted from cells for research. Therefore, the use of in-situ spectroscopic detection and imaging methods to achieve in vivo LLPS analysis is of great value. Optical photothermal infrared (O-PTIR) spectroscopy is a recently developed molecular spectroscopy technique that allows to obtain chemical information at a submicrometric scale. The high spatial resolution (≈ 450 nm), lack of sample preparation, and comparability of the spectral results to traditional Fourier transform infrared spectroscopy make it a promising candidate for the analysis of studying biomolecules, especially for LLPS research [2]. Cryptochromes are a type of photolytic enzyme like protein widely present in higher eukaryotes[3]. They mediate blue light regulation of gene expression in plants to regulate important growth and development processes. In Arabidopsis, the CRY2 protein is its blue light receptor [4], but the specific molecular mechanism is not yet clear. This study focuses on the functional CRY2 protein, and we employed the O-PTIR spectroscopy to investigate the inherent conformational heterogeneity and structural distribution inside the CRY2 protein and its phase separated aggregates, trying to understand the possible mechanism of CRY2 protein's phase separation and photo-response process through comparative analysis of O-PTIR spectroscopy peak positions. This unique method combines the capabilities of vibrational spectroscopy and spectral imaging, providing rich molecular information within the mesoscopic liquid condensation phase at single droplet resolution.

References:

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Oral Presentation

Poster Presentation

In situ Synchronization Single Molecule Force-Infrared Spectroscopy Characterizing of Mechanochemistry

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Mechanochemistry aims at understanding the chemical or physicochemical reaction activated by mechanical load. A large number of mechanophores have been developed for the preparation of stress-responsive smart polymer materials, which provided damage detection, self-healing/reinforced and other functions. Atomic force microscope based single molecule force spectroscopy (AFM-SMFS) allows quantitatively force loading towards a single molecule chain, combining with precision length detection. The extensive force measurement range and test environment compatibility makes AFM-SMFS become one of the most widely used mechanochemistry characterization technique. However, only force and end-to-end distance can be obtained from AFM-SMFS, while the chemical information of the stretched molecule is missing. It requires a large number of *ex situ* chemical characterization methods or simulation to get solid conclusion.

To address this problem, we combine AFM-SMFS with a chemically resolved spectrum, infrared (IR) spectroscopy, expecting to achieve chemical identification of the stretched molecule. After activated by IR laser, the oscillation of stretched molecule can be detected by the AFM tip via a parallel covalent connection strategy[1], and the single molecule IR absorption spectroscopy can be read[2]. The mechanochemical reaction of *gem*-dichlorocyclopropanes (gDCC) can be detected with the SMFS-IR technique. A detectable change at ~ 1660 cm^{-1} (C=C) is observed before and after the contour length increment of SMFS testing. This newly developed spectroscopy technique can provide a new perspective to understanding the mechanical response of systems with complex interactions.

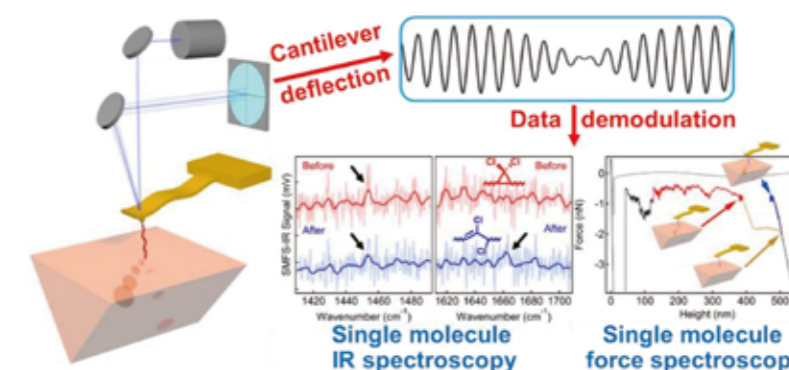


Fig. 1: Single molecule force-infrared correlation spectrum.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

Surface enhanced Raman spectroscopy research on self-supporting MIL-100(Fe)/AgCl/Ag

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Surface Enhanced Raman Spectroscopy (SERS) is an advanced analytical technology, which can enhance the Raman scattering signal of molecules on rough metal surfaces and realize high-sensitivity molecular detection, and is widely used in food environment and catalysis. MIL-100(Fe)/Ag with MOFs structure was constructed on the surface of silver foil by using displacement reaction and liquid phase solvent epitaxy to functionalize the substrate, and then by low temperature cyclic self-assembly. The SERS performance was tested with MB as a probe molecule, using a 633 nm excitation wavelength. Raman peaks at 1624, 1394, and 448 cm⁻¹, characteristic of MB, were detected, revealing the material's high sensitivity and reproducibility. MIL-100(Fe)/AgCl/Ag can detect MB concentrations as low as 4×10⁻⁸ M, attributed to continuous plasmons, synergy between AgCl nanoparticles and Ag foil, and the material's porous structure. SERS spectra of MB, R6G, and norfloxacin demonstrate the substrate's detection capabilities. After photodegradation, the SERS signal decreased, indicating self-cleaning and reusability.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

Two-dimensional sum frequency generation spectra simulation of the water interface based on local quantum vibration embedding to reveal hydrogen bond dynamics at water interfaces

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Interfacial water molecules play a crucial role in surface processes, influencing reaction dynamics significantly. Understanding the dynamics of the hydrogen bonding network at the water interface and its kinetic processes requires not only an in-depth understanding of its interfacial water molecule structure, but also a clear understanding of the rates and mechanisms of energy transfer and dissipation. Two-dimensional vSFG (2D-vSFG) combines time-resolved spectroscopy with surface selectivity, a powerful tool for studying water interface dynamics and molecular vibrations. Developing precise theoretical methods to simulate 2D-vSFG spectra and analyze dynamic changes is significance. In the current theoretical simulation studies of 2D-vSFG spectroscopy, the consideration of quantum effects of molecular vibrations and molecular dynamics environmental factors is still insufficient, and the simulation of dynamical processes involving multiple vibrational modes coupled and multiple quantum states involved is still limited. Local quantum vibration embedding (LQVE) integrates quantum mechanics for specific vibrations with classical dynamics for the system, incorporating weak intermolecular interactions comprehensively. Calculating physical quantities precisely allows rigorous analysis of microstructural dynamics, transition dipole moments, and polarizability. This approach enhances simulation accuracy economically while maintaining high precision. This study applies LQVE to simulate 2D-vSFG spectra of water interfaces, advancing understanding of nonlinear spectroscopy and offering insights into interface dynamics, particularly hydrogen bonds.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

Surface-enhanced Raman scattering of Polyoxometalate-Based Metal Organic Frameworks

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Metal-organic frameworks (MOFs) are characterized by large surface area, high porosity and strong adsorption capacity. Polyoxometalates (POM) are defined as a class of compounds with fixed structures that are easily functionalized and exhibit excellent dispersibility. Due to the modulation of energy levels by POM and MOF composites, it is anticipated that they will synergistically enhance the surface-enhanced Raman scattering (SERS) effect. In this work, we explored the potential of one-step solvothermal process to synthesize H₃PW₁₂O₄₀ (HPW)-CuBTC material [1]. This material has high surface area and abundant activity, showing significant SERS activity. In the case of methylene blue (MB), the detection range is extended from 10⁻⁵ M to 10⁻⁸ M, with a minimum detectable concentration of 3×10⁻⁸ M. The SERS activity is attributed to the synergistic enhancement mechanism of localized surface plasmon resonance (LSPR) and charge transfer (CT). Compared with CuBTC and HPW, the absorption of LSPR at 633 nm is stronger in HPW CuBTC, resulting in a certain EM enhancement effect. In addition, CT also contributes to the SERS effect of the system. The HPW CuBTC substrate is a simple and cost-effective tool that is expected to have significant practical applications in the field of rapid detection based on SERS in the future.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

Application of fs-CARS Technology in Combustion Diagnostics

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In-depth understanding and precise control of the combustion process can help improve the performance of heat engines, so comprehensive and reliable diagnosis to the flames has always been an important research field in combustion research. In high-temperature and high-pressure flames, the reliability of traditional optical diagnostic techniques tends to decrease with the increase of flame temperature due to the effects of broadening and quenching caused by molecular collisions. Spectroscopic techniques based on femtosecond laser pulses have shown potential to overcome this problem. Since the interaction time between femtosecond laser and medium is much shorter than the average time interval of molecular collisions in gas phase, the interference caused by molecular collisions can be eliminated from the measurement.

In this work, we demonstrate the application of femtosecond time-resolved coherent anti-Stokes Raman spectroscopy (fs-CARS) in combustion diagnostics. Using the fs-CARS technology, the information about the flame is obtained by detecting the vibrational relaxation process of the gauge molecules [1]. The temperature and main components of the flame can be accessed with the temperature range and detection sensitivity up to 2500 K and 0.5 μmol/ml. In the temperature measurement experiment, the transient temperature of a methane/air swirl flame was measured with a sampling rate of 100 Hz and an accuracy of 3.7% (fig. 1a) [2]. In the component detection experiment, trace intermediate species such as C₂H₂ and CO were successfully detected in kerosene flame (fig. 1b). These experiments show that the fs-CARS technology is a powerful tool for studying high-temperature combustion processes.

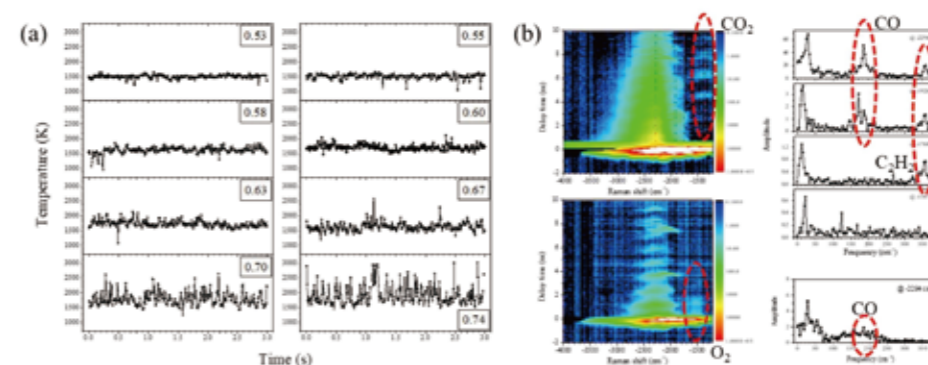


Fig. 1: (a) Evolution of swirl flame temperature at different equivalent ratios. (b) Main components in kerosene flame given by time- and frequency- resolved CARS spectra.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

Synthesis of Aluminium-doped Zinc Oxide Nanomaterials and Atmospheric Window Emissivity Studies in the Infrared Region

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In order to study infrared plasmonic materials with localised surface plasmon resonance (LSPR) properties, we determine the heteroatom doping ratios with respect to the localised surface plasmon resonance doping rate (ITO) and aluminium-doped zinc oxide (AZO) nanomaterials, mainly by tuning different heteroatom doping ratios. In general, the plasma resonance absorption intensity is proportional to the square root of the carrier density. For AZO nanoparticles, we have investigated that different feeding ratios during synthesis affect the final doping of aluminium ions, and that aluminium-doped zinc oxide (AZO) nanomaterials with mid-infrared localised surface plasmon resonance (LSPR) absorption properties are obtained due to the substitution of zinc ions by Al³⁺ in the zinc oxide lattice. We have also explored the potential applications of these nanomaterials, which have been validated in antimicrobial and radiative cooling applications, in addition to enhanced spectroscopy for detection applications. All applications are based on LSPR absorption at long wavelengths (i.e. near/mid infrared). In the future, we may make some progress towards small, medium and mass production for industrial applications.

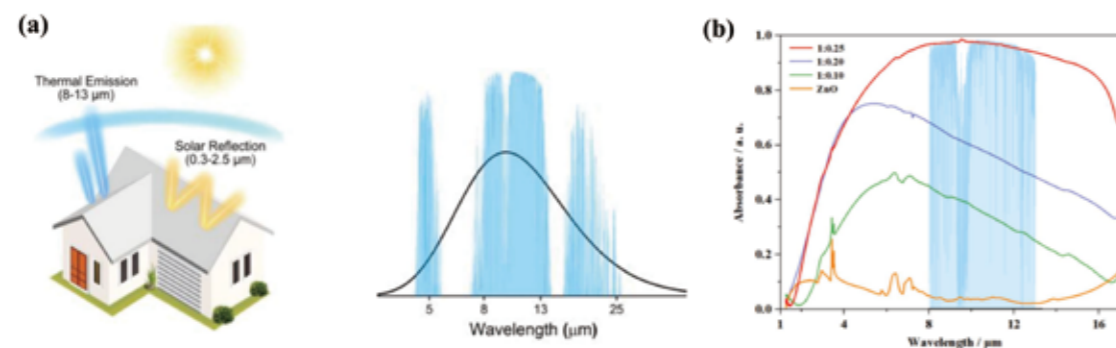


Fig. 1: (a) Atmospheric transmittance(8–25μm) (b) The IR absorption spectra of AZO NPs with different initial doping ratios of Al atoms.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

Micromodulation of methyl formate by supercritical carbon dioxide extraction

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Abstract: Supercritical carbon dioxide (CO₂) extraction is a pivotal technique in industrial purification due to its efficiency and environmental benefits.^[1] This study explores the intermolecular interactions between methyl formate (MF) and CO₂ in the gas phase to understand how these interactions influence the structural and electronic properties of esters.^[2] Using high-resolution microwave spectroscopy and quantum chemical calculations, the MF-(CO₂)_n (n=1-3) clusters have been studied, indicating that CO₂ preferentially interacts with the carbonyl group of MF, rather than self-aggregating. These interactions, primarily tetrel and hydrogen bonds, significantly enhance the stability of the clusters. Notably, the C-O bond length in MF decreases as the concentration of CO₂ increases, demonstrating the modulating effect of supercritical CO₂ on ester structures. This study provides valuable microscopic insights into how CO₂ alters ester structures, offering a foundational understanding of supercritical extraction processes for esters.

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Indicate your choice :

Oral Presentation

Poster Presentation

Surface-Enhanced Raman Scattering and Machine Learning Technique Used for Disease Identification

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Urine is an important physiological sample for the diagnosis of urinary system diseases, and the detection of metabolites in urine can obtain relevant information about diseases. In this study, two surface-enhanced Raman scattering (SERS) probes were constructed by decorating silver nanoparticles with probe molecules (*p*-mercaptobenzoic acid: MBA, *p*-aminothiophenol: PATP), which were used to detect proteins and anions in urine, respectively, to diagnose diseases related to proteinuria and electrolyte imbalance. Using two kinds of sensor probes, urine samples from healthy samples and three kinds of nephritis were tested. According to SERS spectra combined with machine learning technology, differences between healthy urine and nephropathy urine were successfully distinguished, which allowed for the successful diagnosis of nephropathy.

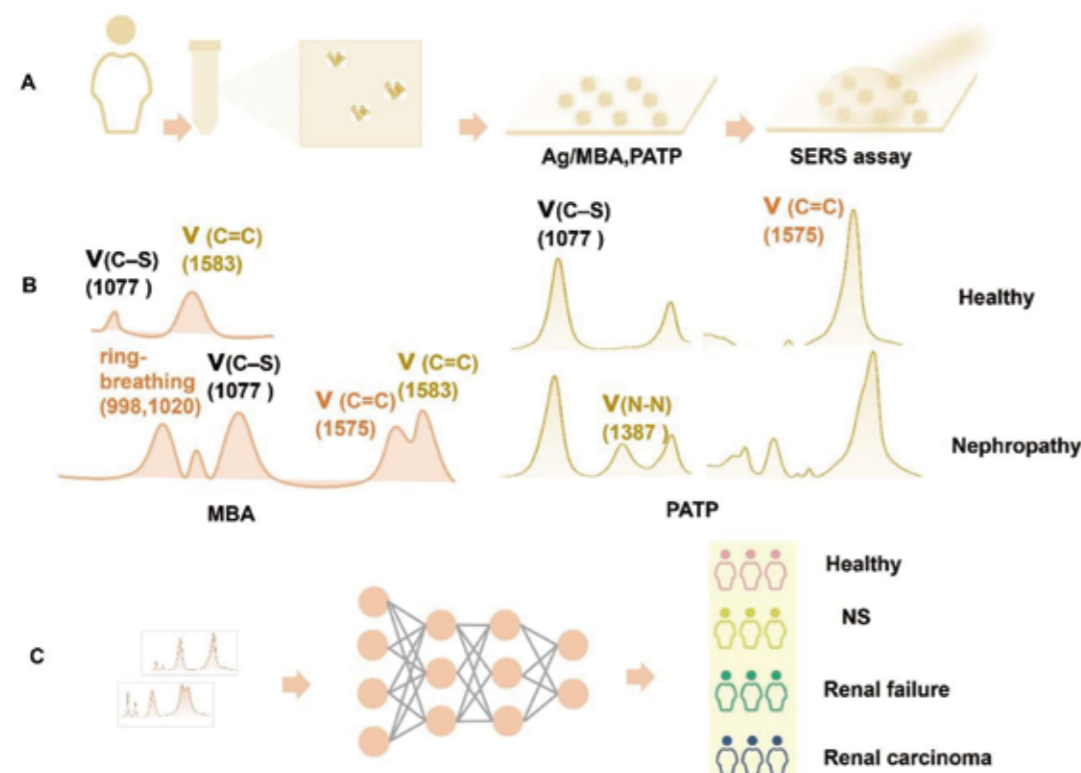


Fig. 1: SERS and machine learning technique used for disease identification

Oral Presentation

Poster Presentation

Two types of water at the poly(methyl methacrylate)/water interface revealed by Time-Resolved Sum-Frequency Generation Vibrational Spectroscopy

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Abstract:

Polymer materials are widely used in coatings, optical fibres, biomedical implants, adhesives and packaging materials due to their unique advantages such as easy modification, easy processing and diversified functions, and have become indispensable and important materials in the national economy. Many macroscopic surface properties that are directly related to the properties of polymeric materials, such as wettability, lubricity, adhesion, biocompatibility and so on, are closely related to interactions between the polymers surface and water molecules.^[1] Poly(methyl methacrylate) (PMMA) is one of the most widely used polymers.^[2] In this study, we investigated the water structure and ultrafast vibrational dynamics of PMMA interfaces using time-resolved sum frequency spectroscopy, and found that there are two different structures of water molecules at PMMA interfaces: One type of water molecule is hydrophilic and has fast vibrational dynamics dominated by strong hydrogen bonds; the other type of water molecule is hydrophobic and has slow vibrational dynamics dominated by weak hydrogen bonds.

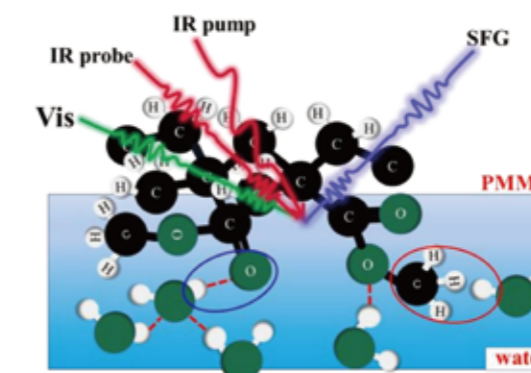


Fig. 1: Proposed molecular model of the PMMA/water interface.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

Construction of two-dimensional metal sulfide-based nanozyme-SERS substrates

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Surface-enhanced Raman scattering (SERS) is an ultra-sensitive molecular detection strategy, some functional nanomaterials can be used as both SERS substrates and nanomimetic enzymes, thus a variety of nanozyme-SERS systems have been constructed, which have been broadly applicable in many fields.^[1-3] Here, NiCo₂S₄@Au nanomaterials were prepared by a hydrothermal and chemical reduction methods with a tuned Au ratio, exhibiting excellent morphology and properties. The special enhanced charge transfer capability property of Ni and Au are the main contribution to its SERS enhancement. As shown in Fig. 1 shows a typical TEM image of the resultant NiCo₂S₄@Au nanomaterials. It can be clearly observed that the Au nanoparticles (NPs) have been successfully deposited on the surface of NiCo₂S₄ nanosheets. NiCo₂S₄@Au nanomaterials can be used as semiconductor SERS substrates for the detection of 1 nM crystal violet probe molecules. Peroxidase-like activity was assessed by the typical color development reaction of 3,3',5,5'-tetramethylbenzidine(TMB) with UV-vis and SERS spectra. This two-dimensional metal sulfide simulated peroxidase-like nanomaterial has important application prospects in analyzing detection, antibacterial properties, and environmental pollutant degradation.

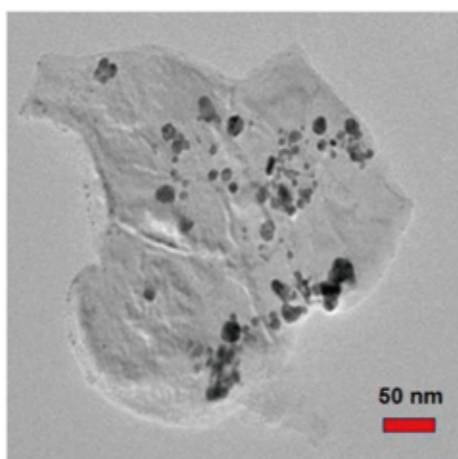


Fig. 1:TEM image of NiCo₂S₄@Au nanomaterials.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

SERS-based Au@CDs with SOD activity for free radical scavenging

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The aim of this study was to develop gold nanoparticles and carbon dots (Au@CDs) composite with superoxide dismutase (SOD) activity and apply it in free radical scavenging assays based on the surface-enhanced Raman scattering (SERS) technique. Excessive accumulation of free radicals in living organisms can cause a variety of diseases, so it is important to develop efficient free radical scavengers and detection techniques. [1]The Au@CDs composite not only possesses excellent SOD mimetic activity, but also significantly enhances the Raman signal. [2] The SERS properties of the composites were investigated by using malachite green (MG) as a detection molecule. The results showed that Au@CD exhibited excellent Raman enhancement in the wavelength range of 200-1800 nm, and the detection limit of MG was up to 10⁻⁸ M, demonstrating extremely high sensitivity and selectivity. In addition, the composite can effectively scavenge superoxide anion radicals in biological systems, suggesting its potential application in biomedical fields. This study provides new ideas for the early detection and treatment of free radical-related diseases and expands new avenues for the application of SERS technology in biomedicine.

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Indicate your choice :

Oral Presentation

Poster Presentation

Synergistic enhancement of ultrahigh SERS activity via $\text{Cu}_2\text{O}@C/\text{Ag}$ yolk shell structure with different cavity thickness

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Nowadays, SERS is being widely applied in many areas because of its potential application in medical diagnosis, biological determination, colloidal and surface chemistry, electrochemistry, and analytical chemistry.^[1] Here, we designed an easily operable layer coating strategy to prepare $\text{Cu}_2\text{O}@Si\text{O}_2/\text{Ag}$ composite nanomaterials with core-shell structure, and then synthesized $\text{Cu}_2\text{O}@C/\text{Ag}$ yolk shell structures with different cavity thickness by calcination and etching for the study of surface-enhanced Raman spectroscopy.^[2] Moreover, the SERS templates showed good stability, the SERS signals almost unchanged after naturally kept for 6 months. Besides, due to the high sensitivity and good stability of the substrates, this work might broaden the potential practical application of SERS.

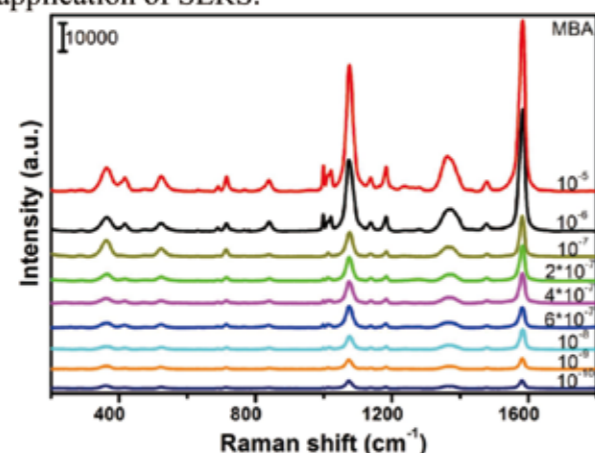


Fig. 1 Concentration-dependent SERS spectra of MBA adsorbed on the $\text{Cu}_2\text{O}@C/\text{Ag}$ yolk shell NPs samples.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

Revealing intracellular lipid droplet microenvironment in pathophysiological events by two-photon fluorescence spectroscopy

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Lipid droplets (LDs) are vital dynamic cellular organelles that maintain lipid equilibrium and support biological communication. The polarity of LDs is critical, as their heterogeneity is closely related to pathophysiological developments. To investigate these changes, we developed a polarity-specific two-photon fluorescence (TPF) platform for real-time and precise monitoring of the polarity microenvironment of intracellular LDs with a carbonized polymer dots (CPD) probe. The polarity of lipid droplets in cells was achieved (Fig. 1). This research enhances the understanding of the correlation between LD polarity and the pathogenesis of various diseases and provides a reference for designing novel LD-targeting probes, in situ fluorescence spectroscopic imaging, and clinical diagnosis of LD-related disorders. Using this platform, we identified differences in LD polarity between cancerous and non-cancerous cells, as well as variations in LD polarity during pathophysiological events such as ferroptosis and steatosis. The development of the CPD probe associated with TPF spectroscopy marks a significant advancement in understanding the role of LDs in lipid-associated diseases.

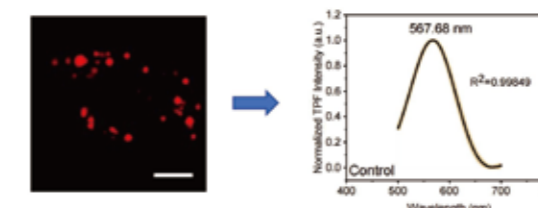


Fig. 1: LD polarity TPF spectra of individual cells

References:

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Oral Presentation

Poster Presentation

Time and Frequency Resolved Infrared Free Induction Decay (IR-FID) of Atmospheric H₂O Observed in Surface Sum-Frequency Generation Vibrational Spectroscopy (SFG-VS)

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In this study, we reported the unexpected observation and mechanistic understanding of the contribution to sum-frequency generation vibrational spectroscopy (SFG-VS) of the gold film surface from gaseous molecules or thin film material molecules in the IR path.^[1] For the case of atmospheric gas, the origin of such unexpected signal is the ro-vibrational coherence of femtosecond coherent infrared free induction decay (IR-FID) radiation from H₂O molecules in the IR path, which was up-converted on gold surface. The up-converted IR-FID signal of gaseous molecules probed by broadband SFG-VS with medium frequency resolution and picosecond time resolution provides a complex frequency and time resolved two-dimensional spectrum (Figure 1), showing the frequency resolved relaxation and rotational coherence of the stretching vibrational molecules. Measuring 2D gaseous H₂O spectra with different temporal resolution and spectral resolution by the visible pulse shaper, helps us obtain information about molecular interactions and dynamic relaxation of H₂O molecules in open air. This FID-SFG method may be used as a sensitive and effective tool for exploring the ro-vibrational dynamics of gaseous and condensed phase molecules in environmental as well as combustion studies, for understanding and controlling these dynamic processes.

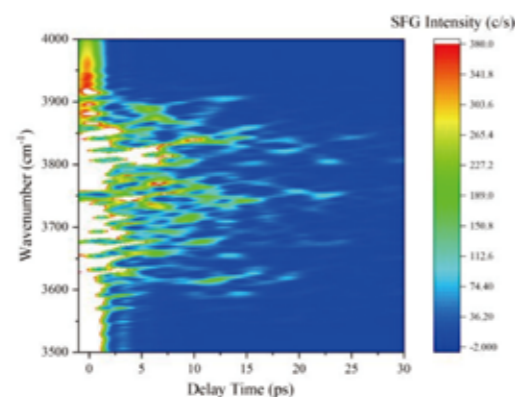


Fig. 1: Time and frequency resolved IR-FID of symmetric and antisymmetric stretching vibrational atmospheric H₂O at air/gold interface.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

The Au@RCDs with core-shell structures were used for in situ SERS detection in biological systems

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In recent years, more and more researches have been conducted on the composite of carbon dots with metals and carbon dots with semiconductors as SERS substrates to improve their SERS properties, optical properties, biocompatibility, etc., and to expand their applications in the study of catalytic reaction mechanisms and the detection of SERS in biological systems with high sensitivity[1,2]. Here, we prepared red emissive carbon dots and designed a red emissive carbon dots/gold nanocomposites (Au@RCDs) with a core-shell structure of about 50 nm in diameter based on the excellent reduction properties of the carbon dots. Due to the synergistic interaction between RCDs and Au, both electromagnetic field enhancement and chemical enhancement are improved, and thus Au@RCDs exhibits a SERS enhancement effect superior to that of Au NPs. The RCDs shell layer makes the material less cytotoxic and more biocompatible, and the small size allows the material to be endocytosed by cells, which provides an unprecedented opportunity to be utilized in biological systems, especially on the cellular level, and it is expected to be a promising candidate for a variety of applications. unprecedented opportunities. The material is expected to be used as an excellent biocompatible substrate for in situ SERS assays in biological systems.

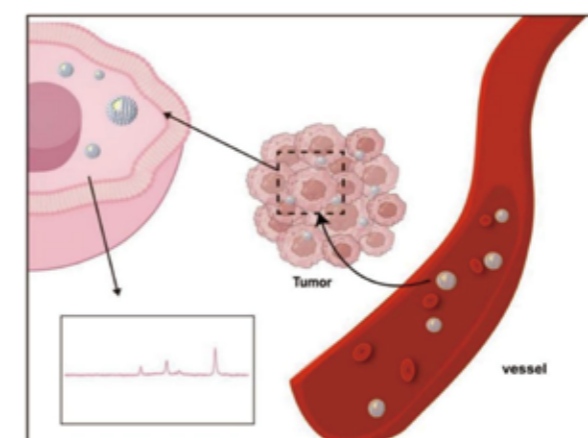


Fig. 1: Schematic representation of Au@RCDs in situ SERS detection in tumor tissue.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

Insights on Z-scheme interfacial charge transfer of TiO₂-NRAs/BiOI-NFs/ Au-NPs nanoheterostructures and unveiling enhanced photoelectrochemical performances

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We synthesized a TiO₂-NRAs/BiOI-NFs/Au-NPs ternary Z-scheme nanoheterostructure using an accessible preparation method. We focused on nanosecond time-resolved transient photoluminescence spectroscopy (NTRT-PL) to characterize the various nanoheterostructures and analyzed the charge transfer (CT) dynamics and carrier fate at their respective interfaces. The ternary nanoheterostructure exhibited superior photoelectrochemical (PEC) performance compared to binary nanoheterostructures, attributed to the synergistic effects of enhanced charge separation and improved injection efficiency. An interfacial charge migration mechanism involving plasmon-induced hot electron injection and transition with oxygen vacancy defects was proposed. The ternary nanohybrids demonstrated a higher photodegradation rate for methyl orange (MO). The TiO₂-NRAs/BiOI-NFs/Au-NPs ternary nanohybrids exhibited a 96.6% photodegradation rate of MO under UV-visible light irradiation, which is 1.47 and 1.19 times that of BiOI-NFs/Au-NPs and TiO₂-NRAs/BiOI-NFs, respectively. Furthermore, the TiO₂-NRAs/BiOI-NFs/Au-NPs ternary nanoheterojunction exhibited the best photodegradation performance under near-infrared light irradiation, with a photodegradation rate 4.3 times and 1.2 times that of the binary TiO₂-NRAs/BiOI-NFs and BiOI-NFs/Au-NPs nanoheterojunction composites, respectively. These findings provide insights into interfacial charge transfer in TiO₂-NRAs/BiOI-NFs/Au-NPs nanoheterostructures and demonstrate their enhanced PEC performances, inspiring the design of high-efficiency and non-toxic Z-scheme heterostructures for various applications.

References:

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Indicate your choice :

Oral Presentation

Poster Presentation

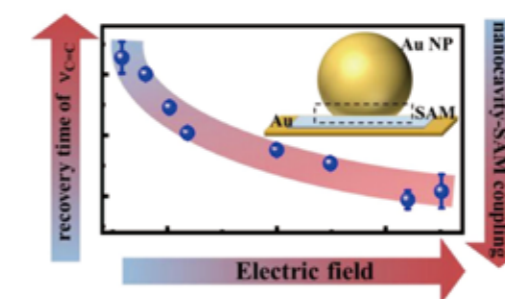
Local Electric Field in Nanocavities Dictates the Vibrational Relaxation Dynamics of Interfacial Molecules

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Plasmonic nanocavities enable the generation of strong light-matter coupling and exhibit great potential in mediating chemical reactions (PMCRs) [1-5]. While an electric field generated by nanocavities (E_n) has recently been reported, its effect on the vibrational energy relaxation (VER) of the molecules in the nanocavities has not been explored [6-10]. In this study, we use self-assembled monolayers of para-substituted thiophenol derivatives on gold films and in plasmonic nanocavities as models [11-12], and reveal the impact of the electric field sensed by the molecules in the nanocavity (E_f) on VER processes for the first time. We determined the magnitudes of E_n and E_f by investigating the bandwidth of the C=C stretching mode ($\nu_{C=C}$) of the phenyl ring via time-resolved femtosecond sum frequency generation vibrational spectroscopy (SFG-VS) supplemented by electrochemical measurements. The magnitude of E_n is almost identical (1.0 ± 0.2 V/nm) beyond the experimental deviation while E_f varies from 0.3 V/nm to 1.7 V/nm depending on the substituent. An exponential correlation between E_f and the complete recovery time of the ground vibrational C=C state (T_2) of phenyl ring is observed. By extending this correlation to the reported macroscopic chemical reactivity (k_{CR}) [13-14], a profound connection between a higher k_{CR} and a smaller T_2 is found. This finding highlights the possibility of regulating vibrational energy flow into a desired reaction coordinate by introducing of rationally designed molecular functionalities within spatially confined nanoscale environments. A molecular-level perspective on the relationship between k_{CR} and E_f and T_2 may aid enriching the current understanding of PMCRs.



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Poster Presentation

Vibration Excitation Dynamics in Nitromethane by First-Principles Molecular Dynamics Simulations

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Understanding the microscopic mechanism of vibrational energy transfer (VET) in energetic materials (EMs) is crucial for their hotspot formation, which is the prerequisite for their macroscopic safety [1]. However, due to the ultrafast process (typically ~ 100 fs to ps) of VET, this poses great challenges for both experimental and theoretical research. Here, we combine density functional theory with non-equilibrium molecular dynamics to selectively excite the C-H stretching vibration in nitromethane (a typical EM), and then track the kinetic energy of the excited and non-excited vibration modes to obtain the law of VET [2-4]. The results indicate that our simulated VET process reproduces the 3D IR-Raman experiment of liquid nitromethane well. In addition, we also found that the coupling between vibration modes depends on the symmetry of the vibration modes, by conducting a short-time Fourier transform on the momentum of the normal vibration mode and using the square of its mode as the spectral energy density [2]. Subsequently, the mode selective excitation dynamics of intramolecular VET in nitromethane molecules indicate the existence of three vibration energy coupling mechanisms: direct symmetric coupling, overtone-assisted coupling, and rotation-assisted coupling [3]. Finally, we found that anharmonic transfers following symmetry rules which involve the couplings assisted by the overtones and rotations, as well as the transfers among the adjacent modes, play important roles in the VET of solid NM by the selective excitations of all 14 intramolecular vibrational modes above 400 cm⁻¹ [4].

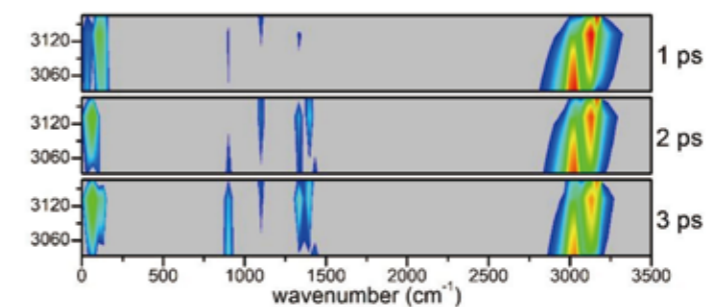


Fig. 1 3D excitation and detected vibrational spectrum of solid nitromethane after the selective excitation of C-H stretching modes and monitoring all the vibrational modes

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Poster Presentation

In Situ Raman Spectroscopy Reveals Cytochrome c Redox Controlled Modulation of Mitochondrial Membrane Permeabilization That Triggers Apoptosis

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The specific interaction between cytochrome c (Cyt c) and cardiolipin (CL) plays a crucial role in the permeabilization of mitochondrial membranes, which is an essential process for the release of apoptosis activators.^{1,2} The structural basis and modulatory mechanism remain incompletely elucidated. Here, we report that Cyt c can induce CL peroxidation independent of reactive oxygen species, which is controlled by its redox states. Moreover, cytochrome c oxidase dysfunction is found to be associated with the initiation of Cyt c redox-controlled membrane permeabilization. To explore the origin of the Cyt c-mediated membrane permeabilization and the underlying modulatory mechanism, we investigate the redox state-controlled unfolding of the protein Cyt c, conformational order of alkyl chains of CL-containing membranes, and the lipid peroxidation by Raman spectroscopy. With the aid of circular dichroism (CD), electron paramagnetic resonance (EPR) spectroscopy, and mass spectrometry, the ROS-independent and Cyt c-redox regulated CL oxidations are studied. The permeabilization-caused membrane pore formation, membrane collapse, and budding are observed by confocal microscopy. Furthermore, initiation of the redox-dependent modulation process is explored by inhibiting cytochrome c oxidase in isolated mitochondria. A modulatory mechanism underlying Cyt c redox-dependent permeabilization is finally proposed. These results confirm the importance of a redox-dependent modulation mechanism in the early stages of apoptosis, which can be exploited for the design of cytochrome c oxidase-targeted apoptotic inducers in cancer therapy.

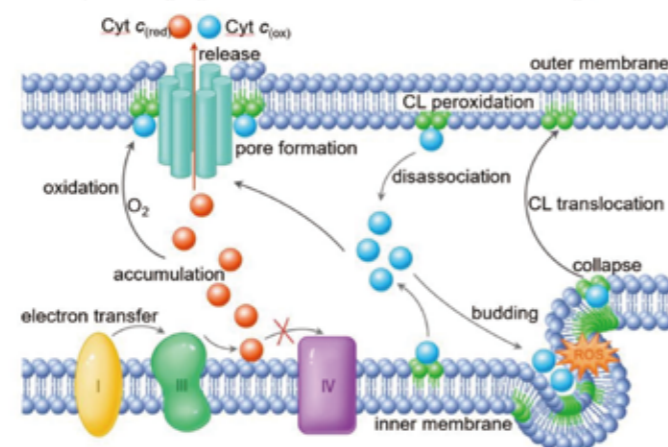


Fig. 1: A Cyt c redox-controlled modulatory mechanism in mitochondria before Cyt c release including Cyt c oxidase inhibition, Cyt c_(red) accumulation, CL peroxidation, membrane pore formation, membrane collapse/budding and CL translocation.

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