ACKNOWLEDGMENTS

The Organizing Committee expresses its gratitude to the Hunan Normal University for hosting this conference and to all the sponsors. Co-host: Zhengzhou University of Light Industry. Supporter: The Hunan Quantum Science & Technology Society. A number of cash prizes, generously provided by Elsevier, will be awarded for the best student posters presented at the conference.

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Scan the QR code to join the conference wechat group “Quantum International Frontiers 2026”.
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Brief overview of
Quantum International Frontiers 2026

This meeting is intended to be the fourth of a series of Quantum International Frontiers conferences. The idea is that the meetings can take place around China and internationally, returning to Changsha for our significant anniversaries, this year being the 88th anniversary of the founding of Hunan Normal University.

For the interested non-Chinese reader: the red and blue intertwined 8's is to signify the 88th anniversary of Hunan Normal University and the rainbow spectrum of the Greek letter psi represents the electromagnetic spectrum.

As you will know by now, the format of the Q.I. Frontier conference series is different from other series, in that in addition to the standard invited lectures, we have introduced **Pedagogic** and **Frontier** lectures. We think this more inclusive and so to facilitate this we have a live question submission system, accessible from PCs, laptops and mobile devices.

Welcome to Changsha, Hunan Province! We all hope you have a splendid and enjoyable conference!

On behalf of the local organizing committee and co-chairs,

Samantha Jenkins.

Professor Samantha Jenkins (苏曼)

http://beaconresearch.org http://www.quantum-int.org/2026/

2023 JSPS Senior Visiting Fellowship (Grant ID: S22083)

2021 Hunan International Science and Technology Cooperation First Class Award(湖南省国际科学技术合作奖)

2020 Xiaoxiang Scholar(潇湘学者)

2013 Chinese Government Friendship Award recipient

2012 6th Xiaoxiang Friendship Award recipient

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College of Chemistry and Chemical Engineering, Hunan Normal University

Changsha, Hunan, The People's Republic of China

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Quantum International Frontiers

October 15-18, 2026

Changsha, China

Scientific programs arranged by day

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Arrangement of the Conference

The Timing and Location of the Conference

- 16th, Oct. 08:30 - 09:00 Opening Ceremony: **Crowne Grand Ballroom（皇冠大宴会厅）**, 6th Floor
- 16th - 17th, Oct. The **Frontiers**/**Pedagogical**/**Invited Lectures** will be given in **Crowne Grand Ballroom（皇冠大宴会厅）**, 6th Floor.
- 18th, Oct. Invited Lectures (**P1**, **P2**, **P3**, **P4**) will be given in **Hibiscus Room（芙蓉厅）**, **Peony VIP Room（牡丹厅）**, **Camphor Room（香樟厅）** and **Azalea Room （杜鹃厅）** respectively in 6th Floor.
- 17th, Oct. 12:00 - 14:00 The Poster Session will be held in **Crowne Grand Ballroom**, 6th Floor

Dining Room of the Conference

15th - 18th, Oct. Lunch and Dinner are provided free of charge during the conference, at the **Taste All Day Dining Restaurant（品味全日餐厅）**, 6th Floor

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Conference Registration

Thursday, 15 October, 2026

14:00 to 18:00
6th Floor, Crowne Plaza Changsha Development Zone

Conference Program

Friday, 16 October, 2026 Crowne Grand Ballroom 皇冠大宴会厅

Chair: Hui jing

08:30 to 09:00
Opening Ceremony, conference photograph

09:00 to 09:30
Elfi Kraka (Southern Methodist University)
From Phonon Bands to Bonds: Wavevector-Resolved and Wannier-Type Local Vibrational Mode Analysis

09:30 to 10:00 **Pedagogical lecture**
Yanqing Lu (Nanjingi University)
Exploring Soft Matter Photonics

10:00 to 10:15 **Tea break**

10:15 to 11:00 **Pedagogical lecture**
Denis Sabirov (Ufa University of Science and Technology)
Polarizability of fullerenes and polycyclic aromatics. From DFT to materials science and astrochemistry

11:00 to 11:30
Cheol Ho Choi (Kyungpook National University)
MRSF-TDDFT and Beyond

11:30 to 12:15 **Pedagogical lecture**

Xiaosong Ma (Nanjing University)

Quantum memory at telecom wavelength using erbium-ion ensembles

12:15 **Lunch**

Chair: Steven R. Kirk

13:30 to 14:30 **Frontier lecture**

Pavlo O. Dral (Xiamen University)

Towards Autonomous Computational Chemistry Research with Al and ML

14:30 to 15:00

Samantha Jenkins (Hunan Normal University)

Low-Attosecond Resolution Electronic and Nuclear Dynamics: How Helical Electron Motion Drives Chiral Asymmetry

15:30 to 15:45 **Tea break**

15:45 to 16:30 **Pedagogical lecture**

Dongqing Wei (Shanghai Jiaotong University)

AI drug with quantum computing

16:30 to 17:00

Yuanhao Mao (Army Engineering University of PLA)

Chiral Laser Gyroscopes Breaking The Lock-in Limit

17:00 to 17:30

Keyu Xia (Nanjing University)

Singularity-enhanced sublinear sensing with linear sensors

17:30 to 18:00 **(Online)**

Sergei Manzhos (Institute Science Tokyo)

Augmenting DFTB with customized interatomic potentials mechanics to facilitate large-scale electronic structure calculations

18:00 **Dinner**

Saturday, 17 October, 2026 Crowne Grand Ballroom 皇冠大宴会厅

Chair: Elfi Kraka

08:00 to 08:30
Yun-Feng Xiao (Peking University)
Ultra-high-Q Microcavity Optics & Photonics

08:30 to 09:00
Junqiu Liu (Shenzhen International Quantum Academy)
Ultralow-loss silicon nitride integrated photonics

09:00 to 10:00 **Frontier Lecture**
Zhonghan Hu (Shandong University)
The Finite Coulomb Lattice Sum

10:00 to 10:15 **Tea break**

10:15 to 10:45
Michał Lesiuk (University of Warsaw)
Rank-reduced coupled cluster theory

10:45 to 11:15
Yang Guo (Shandong University)
Multi-reference Methods for Large Active Spaces and Relativistic effects

11:15 to 12:00 **Pedagogical lecture**
Maxim Gelin（Hangzhou Dianzi University）
Femtosecond nonlinear spectroscopy from the point of view of a theoretician

12:00 **Lunch and Poster Session**

Chair: Ireneusz Grabowski

13:30 to 14:00
Min Zhuang (Shenzhen University)
Quantum lock-in detection with cold atoms

14:00 to 14:30
Yasuteru Shigeta (University of Tsukuba)
An Integrated Computational Chemistry Workflow for Drug Discovery and Protein Function Analysis

14:30 to 15:15 **Pedagogical lecture**
Julia Contreras-García (Sorbonne Université)
Quantum topology: understanding chemistry from 3D fields

15:30 to 15:45 **Tea break**

15:45 to 16:45 **Frontier Lecture**
Tomasz A. Wesolowski (University of Geneva)
Multiplicative embedding potentials for multi-scale simulations of electronic properties: exact properties and approximations

16:45 to 17:30 **Pedagogical lecture**
John M. Herbert (The Ohio State University)
Large-Scale, High-Accuracy Quantum Chemistry via Fragmentation

17:30 to 18:00 **(Online)**
Piotr Piecuch (Michigan State University)
Recent Advances in the CC(P;Q) Formalism: CIPSI-Driven and Adaptive Approaches

18:**00** **Dinner**

Sunday, 18 October, 2026 Hibiscus Room 1+2 (P1) 芙蓉厅 1+2

Chair: John M. Herbert

08:00 to 08:30
Paul W. Ayers (McMaster University)
The Seniority Quantum Number in Many-Body Quantum Mechanics

08:30 to 09:00
William Glover (NYU Shanghai)
Water Catalyzes the Decay of a Ground-State Twisted Intermediate During the Electronic Relaxation of Uracil

09:00 to 09:30
Timothy Hele (University College London)
A Radical Approach to Machine Learning and Electronic Structure Theory

09:30 to 10:00
James Anderson (Universidad Nacional Autónoma de México)
The Impact of Scalar Relativity and Electron Correlation on QTAIM Properties

10:00 to 10:15 **Tea break**

10:15 to 10:45
Ireneusz Grabowski (Nicolaus Copernicus University in Toruń)
An Evaluation and Development of the Hybrid KS DFT Functionals Based on the KS Exchange-Correlation Potentials - the UMK26 hybrid functional.

10:45 to 11:15
Ya-Qian Liu (Zhengzhou University of Light Industry)
Neuromorphic Devices Modulated by Quantum Effects and Ionic Coupling

11:15 to 11:45
Mingyuan Hong (University of Electronic Science and Technology of China)
Multiphoton quantum plasmonic system

12:00 **Lunch**

Chair: James Anderson

13:30 to 14:00

Libor Veis (Czech Academy of Sciences)

Projection-Based DMRG-in-DFT Embedding for Strongly Correlated Molecular Systems

14:00 to 14:30

Michael Dolg (Beijing Normal University)

Investigation of medium-sized methane clusters with quantum chemical first principles and ab initio calculations

14:30 to 15:00

Jin-Lei Wu (Zhengzhou University)

Superadiabatic engineering of quantum state transfer across multi‐state platforms

15:00 to 15:30

Yan Wang (Zhengzhou University of Light Industry)

Liquid photonic-molecule microlasers for ultrasensitive biosensing

15:30 to 15:45 **Tea break**

Sunday, 18 October, 2026 Peony VIP Room (P2) 牡丹厅

Chair: Jianxin Song

08:00 to 08:30
Sidian Li (Shanxi University)
Fluxional Covalent Bonds, Hydrogen Bonds, and Halogen Bonds in Chemistry

08:30 to 09:00
Yonggang Yang (Shanxi University)
Ultrafast charge migration: simulations, manipulations, and applications

09:00 to 09:30
Xinxing Zhou (Hunan Normal University)
Photonic spin Hall effect: Manipulations and applications

09:30 to 10:00
Ya-Ju Song (Hengyang Normal University)
Quantum-Interference Control of Single-Photon Transport and Frequency Conversion in Waveguide QED

10:00 to 10:15 **Tea break**

10:15 to 11:15 **Frontier lecture**
Hong Jiang (Peking University)
Recent developments of density-matrix based quantum embedding approaches to strongly correlated systems

11:15 to 11:45
Dongbo Zhao (Yunnan University)
The Density Knows: Information-Theoretic Learning from Molecular Response to Multiproperty Prediction

12:00 **Lunch**

Chair: Yonggang Yang

13:30 to 14:00
Jianxin Song (Hunan Normal University)
Synthetic Chemistry of Porphyrinoids

14:00 to 14:30
Kaisheng Wang (Hunan Normal University)
Synthesis, Structure, and Properties of π-Extended Porphyrinoids

14:30 to 15:00
Ling Xu (Hunan Normal University)
Chemistry of Subporphyrin Borenium cations

15:00 to 15:30
Mingbo Zhou (Hunan Normal University)
Site-selectivity-enabled novel fused porphyrins: precise synthesis and property investigation

15:30 to 15:45 **Tea break**

Sunday, 18 October, 2026 Camphor Room (P3) 香樟厅

Chair: Xiguang Wang

08:00 to 08:30
Dongping Zhong (Shanghai Jiao Tong University)
Optical coherent control of biological electron transfer

08:30 to 09:00
Chuancun Shu (Central South University)
Quantum Control of Ultracold Molecules: From Quantum States to Quantum Gates

09:00 to 09:30
Yaxin Zhai (Hunan Normal University)
Spin Effects and Spin Control in Hybrid Semiconductors

09:30 to 10:00
Fuxiang Li (Hunan University)
Universal scaling behavior in topological quantum phase transitions under driven critical dynamics

10:00 to 10:15 **Tea break**

10:15 to 10:45
Jian-Sheng Dong (Jishou University)
Magnetoelectric Coupling and Quantum Transport in Two-Dimensional Compensated Magnets

10:45 to 11:15
Qing-Shou Tan (Hunan Institute of Science and Technology)
Reinforcement-learning-assisted nonreciprocal optomechanical gyroscope

11:15 to 11:45
Wenjie Dou (Westlake University)
Memory kernel coupling theory to quantum dynamics

12:00 **Lunch**

Chair: Changliang Ren

13:30 to 14:00

Xiguang Wang (Central South University)
Electrically tunable non-Hermitian magnon propagation in magnetic waveguides

14:00 to 14:30

Qiong Chen (Hunan Normal University)
Robust Quantum Control and Sensing in Defect Spin Systems

14:30 to 15:00

Jianqi Zhang (Chinese Academy of Sciences)
Experimental witness of quantum jump induced highorder Liouvillian exceptional points

15:00 to 15:30

Xiao-Ying Zhou (Hunan University of Science and Technology)
Friedel oscillations in semi-Dirac and altermagnet systems

15:30 to 15:45 **Tea break**

Sunday, 18 October, 2026 Azalea Room (P4) 杜鹃厅

Chair: Rui-Bo Jin

08:00 to 08:30
Jie-Qiao Liao (Hunan Normal University)
Dark Mode and Dark State Theory in Quantum Physics

08:30 to 09:00
Liwei Yu (Nankai University)
Tensor-Network Machine Learning: Trainability, Generalization, and Statistical Structure

09:00 to 09:30
Changliang Ren (Hunan Normal University)
A Unified Framework for Sequential Quantum Correlation Sharing

09:30 to 10:00
Ran Huang (National University of Defense Technology)
Nonreciprocal and non-Hermitian photon blockade effects

10:00 to 10:15 **Tea break**

10:15 to 10:45
Yu-Hong Liu (Hunan First Normal University)
Machine-learning-assisted quantum state engineering in cavity optomechanical systems

10:45 to 11:15
Yong-Qiang Li (Hunan Normal University)
Multi-Parameter Quantum Positioning Schemes for Different Scenarios

11:15 to 11:45
Ji-Bin Yuan (Hengyang Normal University)
Temperature-enhanced quantum sensing

12:00 **Lunch**

Chair: Yaxin Zhai

13:30 to 14:00
Rui-Bo Jin (Hunan Normal University)
Advanced quantum metrology with Hong-Ou-Mandel interferometers

14:00 to 14:30
Yafeng Jiao (Zhengzhou University of Light Industry)
Hybrid Cavity Optomechanics: A Versatile Platform for Manipulating Macroscopic Quantum Entanglement

14:30 to 15:00
Xiaoyan Cao (Beijing Normal University)
New Developments and Applications of Relativistic Energy-consistent Pseudopotentials

15:00 to 15:30
Ye-Xiong Zeng (Hunan Normal University)
Bosonic Quantum Error Correction: Simpler Structures, Stronger Protection

15:30 to 15:45 **Tea break**

Closing Ceremony

Hibiscus Room 1+2 芙蓉厅 1+2

Chair: Samantha Jenkins

16:00 to 16:30
Award the Frontiers Poster Prizes.
See you at Quantum International Frontiers V

Poster Session

Saturday, 17 October, 2026 12:00 Crowne Grand Ballroom 皇冠大宴会厅

Chair: Tianlv Xu

P-001

Zhongyu Liu

Equation-of-motion method and simulation of six-wave-mixing signals of excitionic trimer

P-002

Alireza Lashkaripour

Quintet Mixed-Reference Spin-Flip (QMRSF) Theory: A New Framework for Strong Correlation

P-003

Xinmiao Li

Theoretical study of internal conversion through the prism of six-wave-mixing Spectroscopy

P-004

Weixi Wu

Exploring Singlet Fission Characteristics via Simulations of Six-Wave Mixing Spectroscopy

P-005

Igor Sawicki

Limits of self-consistent Double Hybrid DFT

P-006

Mateusz Witkowski

MERCE - Method-Space Correlation Energy Extrapolation

P-007

Jiawen Kong

Full symmetry-breaking of electronic and nuclear dynamics for low attosecond resolution of electronic chirality

P-008

Jingqin Tu

Low-Attosecond Resolution Electronic and Nuclear Dynamics Revealing the Origin of Chiral Asymmetry: A Consequence of Helical Electron Motion

P-009

Xintao Song

Thermomechanically squeezed multi-mode phonon lasers with levitated optomechanics

P010

Yanzi Jing

Third-Order Exceptional Point and Quantum Squeezing in a Pseudo-Hermitian Semiconductor Optomechanical System

P011

Yan Wang

Spin Bunching Of Conjugated Structured Photons Based On Metasurfaces

P012

Rui Zhang

Enhancing the Sensitivity of Quantum Optomechanical Gyroscope by Optical Kerr Effect

P013

Jinlei Tan

Frequency-space few-photon diode effect

P014

Xuan Zhao

General dark-state theory for arbitrary multilevel quantum systems

P015

Jianxin Song

Efficient ldentification of the lneguivalence of Mutually Unbiased Bases via Finite Operators

P016

Xian-Li Yin

Feedback-enhanced driven-dissipative quantum batteries in waveguide-QED systems

P017

Cheng Liu

Dark-mode theory for quadratic bosonic networks

P018

Hai Zhu

Single-photon scattering in giant-atom topological-waveguide-QED systems

P019

Yi Xu

Simultaneous ground-state cooling of two levitated nanoparticles by coherent scattering

P020

Yusheng Tang

Highly sensitive temperature sensing via quadratic optomechanical coupling

P021

Zeping Liu

Boundary time crystals beyond mean-field theory: A stroboscopic rotating-wave approximation

P022

Jiakang Wu

Manipulating Topological Polaritons in Optomechanical Ladders

P023

Zi'nuo Cai

Complementarity and Correlations in sequential scenario

P024

Li Liu

Crossover between Coherent and Dissipative Synchronization in Cavity Magnonics

P025

Meimei Zhou

Enhanced entanglement of two distant mechanical oscillators in a two-cascaded-cavity optomechanical system via optical parametric amplifier

P026

Mian Mao

Nonreciprocal Microwave Transmission in a Passive-Active Double-Cavity-Magnon System

P027

Yufeng Su

Mpemba effect caused by anomalous heat conduction in a quantum dot system

P028

Ruochen Wang

Enhancing Optomechanical Entanglement and Mechanical Squeezing by theSynergistic Effect of Quadratic Optomechanical Coupling and Coherent Feedback

P029

Yunlan Zuo

Synchronized and anti-synchronized photon blockade

P030

Run Zhou

Mass-Independent Scheme for Enhancing Spatial Superpositions

P031

Jing Li

Phase-tunable photon circulation in a giant Lambda -type atom-waveguide system

P032

Cancan Xing Wenqing Hong

Solar-Driven Photocatalytic Nitrogen Fixation Using Transition-Metal -Doped CovalentOrganic Frameworks

P033

Huangguo Zhou Yunbo Li

Unveiling the Synergistic Mechanism of Transition Metal–Boron Coordination in B_4C_{12}Nanosheets for Electro-and Photocatalytic Nitrogen Fixation

P034

Yangyang Yuan

Chirp-stabilized dissipative charging of a two-level quantum battery

P035

Jian Tang

Robust photon blockade with hybrid molecular optomechanics

Abstracts for lectures

L-001

From Phonon Bands to Bonds: Wavevector-Resolved and Wannier-Type Local Vibrational Mode Analysis

Elfi Kraka

A phonon in a crystalline solid is a quantized lattice vibration, analogous to a molecular vibrational mode. Unlike molecular vibrations, however, phonons are collective excitations that propagate through the crystal as waves characterized by a wavevector k. Their dispersion relations, ω(k), describe how vibrational frequencies evolve across the Brillouin zone and govern thermal transport, mechanical response, and phase stability. At the Γ-point (k = 0), all unit cells vibrate in phase. The crystal behaves like a single large molecule and molecular Local Vibrational Mode Analysis (LMA) and Composition of Normal Modes (CNM) can extract local chemical information from otherwise delocalized normal modes. Beyond Γ, neighboring unit cells acquire relative phase differences, limiting bonding-based interpretation of phonon band structures. We present in this talk k-resolved LMA decomposing phonons into chemically meaningful distortions, e.g., bond stretches, angle bends, and dihedral motions, while k-resolved CNM follows the evolution of vibrational character across the Brillouin zone. Wannier-type LMA transforms this reciprocal-space information into real-space local vibrational modes centered on individual unit cells, leading to bond strengths being encoded in the full phonon dispersion. Applications to polymeric chains, perovskite crystals, diamond, and magnesium iodate under pressure demonstrate how k-resolved and Wannier-type LMA link crystal structure, phonon dispersion, and chemical bonding, providing an intuitive framework for understanding and tuning structure-property relationships in functional materials.

L-002

Exploring Soft Matter Photonics

Yanqing Lu

We introduce Soft Mattonics—soft-matter photonics—as an emerging area dedicated to the comprehensive harnessing of light through programmable soft materials. Liquid crystals (LCs), with their directional molecular order and pronounced optical anisotropy, serve as a quintessential platform within this framework. This review presents a coherent narrative of how LCs have evolved from a scientific curiosity and display medium into a versatile, reconfigurable system for harnessing light. We articulate this progression along five interconnected frontiers: (i) from scalar to vectorial light manipulation, achieving independent control over polarization and phase; (ii) from free-space to in-plane device architectures, enabling integrated and flexible optical routing within soft materials; (iii) from linear to nonlinear regimes, unlocking second-harmonic generation and reconfigurable nonlinear geometric phases; (iv) from spatial to spatiotemporal modulation, allowing sculpting of complex structured wavepackets; and (v) from passive modulation to active emission, where self assembled gain-anisotropy coupling yields tunable lasing and efficient luminescence. Together, these advances demonstrate that LCs cannot only guide and modulate light but also generate it,establishing Soft Mattonics as a versatile, tunable, low-power, and information-centric photonic material platform. This platform is poised to advance adaptive optics, high-capacity communications, wearable and biomedical photonics, and quantum technologies.

L-003

Polarizability of fullerenes and polycyclic aromatics. From DFT to materials science and astrochemistry

Denis Sh. Sabirov

Polarizability is a molecular property that reflects molecule's behavior under external electric fields. It plays an important role in aromatic and polyene systems, such as fullerenes and polycyclic aromatic hydrocarbons (PAHs), owing to their highly responsive and rich π-electron systems. As a computationally accessible molecular property, it exhibits high sensitivity to changes in chemical structure. In this Lecture, we begin with the standard finite-field technique for calculating polarizability tensors and discuss how additivity rules can be applied to derive analytical expressions linking molecular structure with the polarizability features of fullerene derivatives, including fullerene polymers. The relevance of polarizability parameters to various physicochemical processes involving fullerenes and PAHs is then considered. Specifically, we demonstrate how polarizability values can be used to rationalize the efficiencies of fullerene-based organic solar cells, organocatalysts, and molecular switches, as well as the chemical behavior of carbon-rich molecules in the interstellar medium. The primary objective of this Lecture is to bridge the gap between computational data and experimental physical chemistry.

L-004
MRSF-TDDFT and Beyond
Cheol Ho Choi

Mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT) provides a practical and balanced route to electronic excited states with strong multi-configurational character, including bond-breaking processes, radicals, and conical intersections. In this talk, I will discuss recent developments in the MRSF-TDDFT framework and its applications to photochemical and nonadiabatic phenomena, with emphasis on further theory development beyond the standard formulation. These extensions include extended MRSF (EMRSF) approaches for improving the flexibility and balance of the spin-flip description, QMRSF-DK for strong-correlation problems such as linked singlet-fission states, and MRSF-TDDFTB as an efficient semiempirical route for larger molecular systems and dynamics applications. Particular emphasis will be placed on the accurate description of ground- and excited-state potential energy surfaces, analytic gradients, response properties, nonadiabatic couplings, and their integration into practical computational workflows. I will also describe ongoing efforts toward improved dynamical correlation, efficient dynamics simulations, and open-source implementations for broader community use. These developments aim to make reliable excited-state simulations more accessible for complex molecular systems and photochemical mechanisms.

L-005
Low-Attosecond Resolution Electronic and Nuclear Dynamics: How Helical Electron Motion Drives Chiral Asymmetry
Samantha Jenkins

Controlling and observing electron motion in chiral molecules is a fundamental challenge spanning chemical synthesis, materials science, and spintronics. The electronic origin of chiral asymmetry is revealed by combining real-space analysis of the total electronic charge density with time-dependent density functional theory (DFT) electron-nuclear dynamics simulations in partnership with Next Generation Quantum Theory of Atoms in Molecules (NG-QTAIM). Using simulated ultrafast circularly polarized laser pulses, the correct enantiomeric assignment for (*S*)-1-chloro-1-fluoroethane is demonstrated. Modulating the carrier envelope phase (CEP) angle altered the so-called extrinsic electronic chirality in both chiral (*S*)-1-chloro-1-fluoroethane and achiral chloroethane. Helical bound electron motion, quantified as intrinsic electronic chirality, however, was uniquely observed in the structurally chiral molecule and tuned to induce a significant degree of electronic achiral character via CEP variation. Furthermore, eigenvector-space trajectories exhibited distinct 3-D and 1-D morphologies for chiral (*S*)-1-chloro-1-fluoroethane and achiral chloroethane, respectively. This framework provides the molecular-level design principles needed to transition from static structural descriptors to dynamic electronic properties that can directly impact future practical applications, particularly in asymmetric synthesis and the design of next-generation chiral materials, such as those that exploit the Chirality-Induced Spin Selectivity (CISS) effect.

L-006
Pavlo O. Dral

learning (ML) - the very tool of Al we actually used in AlQM1), in school, I was fascinated by nature and was learning about it as much as I could. I quickly realized that it is impossible to learn everything I am interested in. The more I thought about it, the more obvious was to me that the human mind is just incapable of coping with all the information, which humanity generated, and this is likely to impose a natural barrier on how we can actually make a qualitative jump in our understanding of the world. Computers, in the long run, may overcome this barrier as they are not limited by biological constraints and can have access to all digitalized information. However, can computers by themselves make a qualitative jump in our understanding of nature? This is the first question.

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Later, already in the university doing my master degree, I have had to run many quantum chemical (QC) simulations. It was exciting at first to witness how a computer can predict correctly, e.g., the geometry of a water molecule, but after I run many such simulations, I realized that many of them are quite repetitive and the second question is: can computers by themselves perform all these simulations, analyze results and write papers?

L-007
Quantum memory at telecom wavelength using erbium-ion ensembles
Xiaosong Ma

Quantum teleportation is one of the most important protocols in quantum communication and quantum information. The distribution of quantum states via quantum teleportation is a key ingredient for realizing the quantum internet. In order to integrate such quantum networks into existing fiber networks, entangled photons and quantum memories at telecom wavelength are necessary. Erbium is the ion of choice for this task, given that its optical transitions sit exactly within the C-band, offering the lowest photon loss in propagation. Recently, 167Er ions have been identified as a promising candidate for an efficient, broadband quantum memory at telecom wavelength. However, to date, the quantum teleportation from telecom photons to a solid-state quantum memory based on $167Er^{3+}$ ions, has remained elusive. In this work, we experimentally demonstrate the quantum state teleportation from telecom photons to a solid-state quantum memory based on erbium-ion ensembles. Combining the naturally linewidth of the entangled photons generated from an integrated photonic chip and long life time of $167Er^{3+}$ ions, we realize a storage time of more than 2us. Using quantum-state-tomography and quantum-process-tomography protocols, we obtain an average quantum state fidelity of 81.8% and a quantum process fidelity of 73.6%, which significantly exceeds the classical bound.

L-008
AI drug with quantum computing
Dongqing Wei

Conventional drug discovery faces inherent limitation including long cycles, high costs, and low success rates. Classical computing faces fundamental limitations in dealing with molecular electronic structures, simulating microscopic intermolecular interactions, and resolving complex dynamics or high-dimensional biological systems. Quantum computing provides a new technical route to address the above critical computational challenges through its unique features such as quantum superposition, entanglement, and interference. We present the fundamental principles of quantum computing, its global development landscape, and its applications across core computational stages of drug discovery, covering target identification, molecular simulation, compound screening, ADMET property prediction, and clinical trial optimization. It further analyzes the major challenges currently faced by quantum computing and discusses future trends as deep integration with artificial intelligence, breakthroughs in dedicated hardware technologies, and collaborative construction of the industrial ecosystem. On this basis and in light of the increased computational demands arising from the complex "multi-component, multi-target, systemic regulation" paradigm of traditional Chinese medicine, we explore the innovative applications of quantum computing in this context and proposes a novel heterogeneous computing paradigm characterized by “hierarchical fusion and scenario-driven implementation” aiming to provide new insight for the modernization and precision development of TCM(Traditional Chinese Medicine). Overall, quantum computing holds the promise to surpass the classical capability boundaries of classical computing limits, and accelerating the evolution of drug discovery from the traditional model of empirical trial-and-error and localized intervention toward a new paradigm of precise design and systemic regulation. We shall show also some of the recent progresses we made on AI drug screening in the context of TCM.

L-009
Chiral Laser Gyroscopes Breaking The Lock-in Limit
Yuanhao Mao

The ring laser gyroscope (RLG) has long been a cornerstone of ultra-high-precision inertial navigation, autonomous platforms, and fundamental science facilities, measuring rotation via the Sagnac effect—a minute frequency difference between two counterpropagating beams. Yet an intrinsic limitation, the lock-in phenomenon, suppresses this signal at low rotation rates, preventing broader adoption. Previous remedies, including mechanical dithering and magneto-optic non-reciprocity, rely on external components that hinder miniaturization.
This talk presents a self-biased RLG based on chiral spontaneous symmetry breaking (SSB). In a single-isotope ^{20}Ne-filled He-Ne ring cavity, clockwise and counterclockwise modes compete for gain via overlapping hole burning, inducing strong nonlinear coupling. When the coupling exceeds a critical threshold, the system spontaneously enters a chiral SSB state: one beam intensifies while the other weakens. The resulting intensity asymmetry generates a stable frequency bias through nonlinear frequency pulling, completely eliminating the lock-in region. We demonstrate deterministic chirality switching synchronized with rotation direction and achieve a linear frequency response near zero rotation, with an open-loop bias instability of 2.2×10^{-2} °/h.
Following the spirit of Hilbert's Sixth Problem, we further trace the origin of controllable chiral SSB from Newtonian mechanics of elastic and inelastic atomic collisions, revealing that the emergence of chirality in the He-Ne system is fundamentally a macroscopic manifestation of light-matter interaction governed by gas gain medium dynamics.
In quantum precision measurement, nonlinear effects are often regarded as noise. Our work harnesses them to fundamentally overcome the lock-in effect without external intervention. This paradigm paves the way for fully solid-state, chip-scale laser gyroscopes with transformative potential in commercial aerospace, unmanned systems, and deep-space exploration.

L-010
Singularity-enhanced sublinear sensing with linear sensors
Keyu Xia

Sensing with high sensitivity is of importance for fundamental science and modern high technologies. Since a non-Hermitian system exhibits sublinear response near the exceptional point, where the derivation of the response with respect to perturbation displays a singularity point, it is attracting great attention for exceptional-point-enhanced sensitivity. This presentation will show sensing with sublinear response and enhanced sensitivity by using non-Hermitian and Hermitian linear systems. The sensitivity enhancement in comparison with a Hermitian sensor operating at the diabolic point will be discussed in both the classical and quantum regimes. The results will open a new door for developing ultrasensitive sensors.

L-011
Augmenting DFTB with customized interatomic potentials to facilitate large-scale electronic structure calculations
Sergei Manzhos

Density functional tight binding (DFTB) is attractive for large scale-electronic structure calculations, in particular of molecular and ceramic systems, but requires Slater-Koster (SK) parameters for all atom pairs. Parameters for some atomic pairs may be unavailable or not sufficiently accurate. Interactions between some atomic pairs can be replaced or supplemented with full-range interatomic potentials with minimal effect on the accuracy of structures and band structure. It is effectively QM/MM by type of interaction. The approach, called DFTB-MM, has the potential to simplify or even enable large-scale calculations and is also useful for the calculations of optical spectra. We will present recent results demonstrating its applicability to molecule-nanoparticle (NP) systems.

L-012
Ultra-high-Q Microcavity Optics & Photonics
Yun-Feng Xiao

Ultrahigh-Q optical microcavities confine photons for long periods in small mode volumes, providing a powerful platform for enhancing interactions between light, matter, and mechanical motion. In the first part of this talk, I will discuss optomechanical quantum control in optical microcavities. In the second part, I will focus on microcavity sensing and precision measurement, with particular emphasis on mechanisms that improve both sensitivity and specificity. I will introduce label-free techniques capable of detecting individual nanoparticles, viruses, and molecules, and discuss how microcavity sensing can progress from detection to identification. Finally, I will present the measurement of acoustic vibrational fingerprints of individual cells, opening a previously inaccessible megahertz-to-gigahertz spectral window for single-cell characterization.

L-013
Ultralow-loss silicon nitride integrated photonics
Junqiu Liu

The synthesis, distribution and processing of optical signals are foundational to our modern information society. Presently, conventional fiber and free-space optical technologies face mounting pressure to deliver higher performance within strict size, weight, and power (SWaP) constraints. Driven by advances in CMOS manufacturing and emerging materials, integrated photonics has matured into a transformative platform, enabling the on-chip generation, modulation, and detection of light to overcome the bottlenecks of modern optical communications and data centers. Among the leading material platforms, silicon nitride has emerged as a leading platform, distinguished by its broad transparency window and ultralow optical loss. This talk will highlight recent major advancements in ultralow-loss silicon nitride integrated photonics, focusing on breakthroughs and key applications pioneered by our research group over the past five years.

L-014
The Finite Coulomb Lattice Sum
Zhonghan Hu

The computation of the Coulomb lattice sum, historically known as the Madelung series, is a problem dating back over a century. Its direct-sum evaluation is complicated by the conditional convergence of the lattice sums. The necessity of a rigorous mathematical treatment was first recognized by Redlack and Grindlay, and subsequent derivations by De Leeuw, Perram, and Smith introduced shape-dependent terms for infinite crystals. Yet, a truly analytical understanding of both shape-dependent and finite-size effects for finite crystals has remained elusive.
In this talk, I will present a recently developed lattice summation method for finite crystals of exact shape **s** and size p. This finite lattice sum takes a pairwise formulation for each displacement vector **r** and cleanly decomposes the Madelung series into three distinct components: a bulk term $v_{\mathrm{pbc}}(\mathbf{r})$, which is a periodic function of **r**; a shape-dependent but size-independent non-periodic boundary term $v_{\mathrm{b}}(\mathbf{r}|\mathbf{s})$; and a finite-size correction term $v_{\mathrm{corr}}(\mathbf{r},p|\mathbf{s})$, whose leading-order term decays as $(2p+1)^{-2}$. By analytically isolating the boundary and finite-size corrections within the pairwise formulation, we obtain a rapidly convergent directsummation scheme that remains accurate even for the smallest supercells (e.g., 3^3 unit cells in a regular shape), thereby enabling hands-on calculations of Madelung constants for arbitrary ionic crystals.

L-015
Rank-reduced coupled cluster theory
Michał Lesiuk

In this talk, recent advances in the development of approximate rank-reduced coupled cluster models based on tensor decomposition techniques will be presented. In particular, we will focus on the gold standard CCSD(T) variant. The overall concept of the rank-reduced methodology will be introduced first, outlining the motivation behind the development of this class of approaches and describing how they fit within the broader landscape of quantum-chemical methods, especially when combined with embedding techniques. The principal advantages of rank-reduced theories compared to their canonical counterparts will be demonstrated through specific examples. It will be shown that by systematically applying tensor decomposition to various quantities that appear in the standard formulation of coupled cluster theory, one can substantially reduce both the scaling of computational costs with system size and the associated memory and storage requirements. As a result, the application of rank-reduced techniques makes it possible to significantly extend the range of applicability of the parent methods to larger and more complex systems that would otherwise be computationally prohibitive. Moreover, with proper adjustment of thresholds, errors introduced by the applied rank reduction are typically well below 1 kJ/mol, and therefore chemically insignificant for the vast majority of applications. Recent extensions of this family of methods to the description of excited states in molecular systems, as well as to the time-dependent regime, will also be briefly reviewed to highlight ongoing developments and future directions in this area.

L-016
Multi-reference Methods for Large Active Spaces and Relativistic effects
Yang Guo

Multi-reference (MR) methods are extensively employed to investigate the electronic structures of strongly correlated systems. Among these, multi-reference perturbation theories—particularly Complete Active Space Second-Order Perturbation Theory (CASPT2) and N-Electron Valence State Second-Order Perturbation Theory (NEVPT2)—are the most widely utilized. However, conventional MR methods are typically limited to systems with approximately 15 active electrons and orbitals. To extend the applicability of MR approaches to larger active spaces, an improved formulation known as Full-Rank (FR) NEVPT2 has been developed. When combined with a selected configuration interaction reference, the FR-NEVPT2 method can treat active spaces comprising up to 34 electrons and orbitals while maintaining accuracy comparable to that of conventional NEVPT2. To further enable the treatment of even larger active spaces, it is essential to eliminate the reliance of NEVPT2 on fifth-order reduced density matrices (RDMs). To this end, we propose the NEVPT within Singles (NEVPTS) approximation, which offers computational efficiency superior to NEVPT2 while preserving comparable accuracy. Additionally, extensions of MR methods to incorporate relativistic effects will be discussed.

L-017
Femtosecond nonlinear spectroscopy from the point of view of a theoretician
Maxim Gelin

Nonlinear femtosecond optical spectroscopy comprises a family of techniques such as fluorescence up-conversion, pump-probe, transient grating, photon echo, coherent anti-Stokes-Raman scattering, etc. These techniques differ in the number, ordering, and phase-matching directions of the pulses involved and in the specific information they deliver on the material system under study.
I will present a personal perspective of the development of nonlinear femtosecond spectroscopy from the point of view of a theoretician. Focusing on transient absorption pump-probe spectroscopy and three-pulse photon-echo two-dimensional (2D) spectroscopy, I will clarify the information content of these techniques and demonstrate how the dynamic of the material system under study can be uncovered from measured time- and frequency resolved signals. Finally, I will briefly touch upon modern extensions of nonlinear femtosecond spectroscopy, such as six-wave-mixing spectroscopy, strong-field spectroscopy, and quantum light spectroscopy.

L-018
Quantum lock-in detection with cold atoms
Min Zhuang

High-precision measurement of weak alternating signals in noise background is important for both fundamental science and practical technology. Generally, the target signal is submerged in noise background and is hard to be detected. To obtain a high signal-to-noise ratio, one can decreasing the effect of noise and enhancing the response to the target signal. In metrology, lock-in amplifiers can extract time-dependent alternating signals from an extreme noisy background and have been applied in various fields. However, to the best of our knowledge, all existing studies of quantum lock-in amplifiers concentrate on single-particle systems. Meanwhile, as the target signal usually has an unknown initial phase, it is a challenge to extract the complete information of the target signal (amplitude, frequency and phase).
In this presentation, we present a general protocol for achieving a many-body quantum lock-in amplifier via quatum interferometry under a periodic multipulse sequence. we employ entanglement to enhance the quantum lock-in amplifier and experimentally demonstrate it . Further, we present a general protocol for achieving a quantum double lock-in amplifier via two quantum interferometry with two orthogonal periodic multi-pulse sequences to obtain the complete information of the target signal. We also discuss the experimental feasibility of the two protocols in cold atoms. To save experimental resources, we present a general protocol for achieving a quantum double lock-in detection just via only a single quantum interferometry under sequential orthogonal periodic multipulse sequences. Our study opens an avenue for extracting an alternating signal within strong noise background, which is beneficial for developing practical quantum sensing technologies.

L-019
An Integrated Computational Chemistry Workflow for Drug Discovery and Protein Function Analysis
Yasuteru Shigeta

Computational chemistry has become indispensable for protein function analysis and drug discovery. However, conventional molecular dynamics (MD) simulations face significant challenges, including limited accessible timescales (typically microseconds) relative to biological functions and an inability to describe chemical reactions with standard force fields. To address these limitations, this research presents an integrated computational workflow that combines enhanced sampling techniques with quantum mechanical (QM) descriptions.
Central to this approach is Parallel Cascade Selection Molecular Dynamics (PaCS-MD), which accelerates the exploration of conformational transitions and protein folding problems. For high-precision interaction analysis, the Fragment Molecular Orbital (FMO) method is used to quantitatively evaluate residue-residue and protein-ligand binding energies at the quantum-chemical level, providing superior accuracy over classical molecular mechanics. We utilize the PaCS-MD for flexible docking and estimate the binding energy by FMO to explore the appropriate docking pose.
A major highlight of this work is the development of PaCS-Q, a novel toolkit designed for path sampling in both MD and QM/MM MD simulations. PaCS-Q enables the unbiased, time-resolved exploration of complex biochemical reactions by integrating quantum-level accuracy into the PaCS-MD framework. This allows for the direct observation of bond formation and cleavage without the need for predefined reaction coordinates. The practical utility of these methods is demonstrated in SARS-CoV-2 drug discovery efforts, specifically by analyzing the inhibitory mechanisms of repurposed drugs such as Lopinavir and Ritonavir. Additionally, PaCS-Q has identified transition state structures in enzymatic processes, such as the Claisen rearrangement from chorismate to prephenate, successfully. This integrated methodology offers a powerful platform for bridging the gap between computational simulations and biological reality.

L-020
Quantum topology: understanding chemistry from 3D fields
Julia Contreras-García

Chemical bonding is one of the most fundamental concepts in chemistry, governing the structure, properties, and reactivity of matter. However, despite its central role, the question "what is a chemical bond?" remains open due to the absence of a unique definition and the complexity of its underlying physical nature. Quantum topology provides a powerful framework to address this challenge by extracting chemical information from three-dimensional scalar fields, such as electron density distributions obtained from experiments or quantum mechanical calculations. As a key component of quantum crystallography, topological approaches analyze the organization, localization, and connectivity of electron density to reveal the nature of interactions between atoms and molecules. This class will introduce the principles behind the topological analysis of quantum fields and demonstrate how concepts such as critical points, electron localization, and density-based descriptors provide a direct link between quantum mechanics and chemical intuition. By visualizing and interpreting bonding patterns beyond traditional structural representations, quantum topology offers a new perspective for understanding molecular architectures, crystal structures, and the physical origin of chemical properties.

L-021
Multiplicative embedding potentials for multi-scale simulations of electronic properties: exact properties and approximations
Tomasz A. Wesolowski

One of possible strategies to formulate quantum embedding problem is based on constrained optimization of electron density via the minimzation of the Hohenberg-Kohn energy functional. Such minimization corresponds to the Euler-Lagrange equation taking the form of a Schrödinger equation featuring a multiplicative embedding potential. In the first part, we present the exact relations (Frozen-Density Embedding Theory, FDET) involving the quantities in the Euler-Lagrange equation for embedded wavefunction and for various treatments of electron correlation. In the second part, we make a brief overview of applications of the FDET eigenvalue equation in various multi-level simulation methods developed by us and by others. In the third part, we present our recent applications of the FDET eigenvalue equation for properties for which common semi-local approximants for the FDET embedding potential fail such as charge transfer to solvent excitations or species embedded in environments comprising cations.

L-022
Large-Scale, High-Accuracy Quantum Chemistry via Fragmentation
John M. Herbert

Fragment-based quantum chemistry offers the possibility to defeat the nonlinear scaling of electronic structure calculations for large systems, via distributed parallelization. Its facile implementation has attracted significant interest but convergence with respect to a well-defined level of theory has not always been carefully examined, controlled, or achieved. This talk will describe the development and implementation of fragment-based quantum chemistry methods that do address convergence and that are designed for high-fidelity calculations at levels of theory ranging from semi-empirical methods to density-functional theory to correlated wave functions, in high-quality basis sets. Applications to large-scale enzymatic thermochemistry and protein–ligand binding will be presented, using high-order many-body expansions.

L-023

Recent Advances in the CC(P ; Q) Formalism: CIPSI-Driven and Adaptive Approaches

Piotr Piecuch*

One of the biggest challenges in the coupled-cluster (CC) theory and its equation-of-motion (EOM) and linear-response extensions to excited electronic states has been designing efficient ways of incorporating higher–than–two-body components of the cluster and EOM excitation operators capable of producing accurate energetics equivalent to high-level CC/EOMCC calculations, such as CCSDT, CCSDTQ, and EOMCCSDT, at small fractions of the computational costs, even when electronic quasi-degeneracies become larger and higher–than–two-body components of the cluster and EOM excitation operators become nonperturbative. This challenge can be addressed by adopting biorthogonal moment expansions defining the CC(*P*;*Q*) formalism, which can be viewed as a generalization of the previously developed completely renormalized CC and EOMCC approaches to unconventional truncations in the cluster and EOM excitation operators. For the CC(*P*;*Q*) formalism to be effective, an efficient method must be developed to identify the leading higher–than–doubly excited determinants for inclusion in the subspace of the many-electron Hilbert space used in the iterative steps of the CC(*P*;*Q*) algorithm. This can be done with the help of active orbitals, resulting in the CC(t;3), CC(t,q;3), CC(t,q;3,4), *etc.* hierarchy and its recent extension to open shells via the electron-attachment and ionization-potential formalisms, Quantum Monte Carlo (QMC) wave function propagations employing the configuration interaction (CI) QMC and CCMC approaches, resulting in the semi-stochastic CC(*P*;*Q*) theories, sequences of Hamiltonian diagonalizations originating from the selected CI schemes, such as CIPSI, resulting in the CIPSI-driven CC(*P*;*Q*) algorithms, and the adaptive, self-improving, CC(*P*;*Q*) framework, which frees us from the user-defined active orbitals and non-CC (CIQMC, CIPSI) or stochastic (CIQMC, CCMC) concepts by taking advantage of the intrinsic mathematical structure of the CC(*P*;*Q*) moment expansions in defining the underlying excitation manifolds. In this talk, we will discuss our recent progress in the CC(*P*;*Q*) methodology, especially in the CIPSI-driven and adaptive CC(*P*;*Q*) algorithms and their extensions to excited states. The usefulness of the CIPSI-driven and adaptive CC(*P*;*Q*) methodologies will be illustrated by chemical bond dissociations and reaction pathways, singlet–triplet gaps in biradicals, and excited states including one- as well as many-electron transitions. Information about the CC(*P*;*Q*) methods in GAMESS and our open-source CCpy package available on GitHub at https://github.com/piecuch-group/ccpy, which is an official extension module of PySCF, will be provided as well.

L-P1001
The Seniority Quantum Number in Many-Body Quantum Mechanics
Paul W. Ayers

The seniority quantum number is the number of unpaired fermions in a many-body wavefunction. While it is not a new concept—it's prehistory dates back at least to the 1950s—it is only relatively recently that seniority-based approaches to the quantum many-body problem have been systematically explored. The intrigue of seniority-based methods arises because the seniority-zero configuration interaction (sen0-CI), which is the exact wavefunction in the seniority-zero subspace, is a size-consistent selected CI method and often (but not always) captures strong electron correlation. Remarkably, sen0-CI can often be approximated very accurately by low-cost wavefunctions. We will show that this is not that surprising: every seniority-zero state can be written as a (number-symmetry-broken-and-projected) product of quasiparticles. (This result extends, albeit in an impractical way, to arbitrary-seniority states. It extends, in a more practical way, to bosons.)
While treating seniority-zero states is often computationally facile, most real systems do not preserve the seniority quantum number. We show how to map real Hamiltonians to seniority-zero Hamiltonians (which are then easy to treat). The inverse mapping effectively treats the residual correlation from a seniority-zero description.

L-P1002
Water Catalyzes the Decay of a Ground-State Twisted Intermediate During the Electronic Relaxation of Uracil
William J. Glover

Studying nucleobase response to UV excitation is key to understanding DNA photodamage mechanisms and nature's selection of canonical bases. Seminal work by Bern Kohler showed nucleobases undergo ultrafast non-adiabatic transitions (<1 ps) to the ground state via photoquenching (the sunscreen effect). However, recovery of ground-state bleach spectra for pyrimidines (Uracil, Thymine, Cytosine) was incomplete on <1 ps timescales, showing long-lived components (10–100s ps) initially assigned to nπ* states. This assignment was recently overturned by the discovery of a C5–C6 twisted ground-state intermediate responsible for long-lived transient signals. The intermediate decays over 10–100s ps depending on base, ribose attachment, and solvent, and is implicated in photohydration. To understand the solvent effect, we explored uracil's twisted intermediate decay using QM/MM ab initio molecular dynamics with our FlexiBLE boundary approach. We identified specific solvent interactions catalyzing intermediate decay. Guided by the QM/MM results, we developed a microsolvated model at the DLPNO-CCSD(T)/cc-pVQZ level. Applying harmonic transition state theory yielded near-quantitative agreement with experimental lifetimes and explains the observed kinetic isotope effect. This combination of QM/MM dynamics and microsolvated models for aqueous reaction discovery shows promise at explaining decay lifetimes and photohydration mechanisms for the components of nucleic acids, helping rationalize nucleobase photostability and evolutionary selection.

L-P1003
A Radical Approach to Machine Learning and Electronic Structure Theory
Timothy J. H. Hele

Recent years have seen an explosion of interest in organic radicals due to their high efficiency in organic light-emitting diodes (OLEDs), and their potential for photon upconversion and use in qubits. However, modelling their electronic structure is challenging due to the large size of the molecules, their multireference electronic structure, and the spin contamination problem which can arise from multiple unpaired electrons in the excited states. In this presentation I will present ExROPPP, which we believe is the fastest known method for radical excited state computation, has accuracy comparable to high-level multiconfigurational calculations, and in spin-pure [1]. In addition, alternacy or pseudoparity rules for ground-state closed shell radicals had been derived in the 1950s by Pariser, Parr and Pople but there was no extension to radicals due to the algebraic complexity. In deriving ExROPPP we (Green and Hele) also derived alternacy or pseudoparity rules for the excited states of hydrocarbons radicals, showing their excited states also have 'plus' and 'minus' forms. I will then show what we believe is the first example of machine learning directly from the excited states of radicals where we extend ExROPPP to molecules also containing nitrogen and chlorine by learning the optimal parameters from experimental absorption data and

molecular structures. These breakthroughs pave the way for the high throughput discovery of the next generation of radical-based optoelectronics.

L-P1004
The Impact of Scalar Relativity and Electron Correlation on QTAIM Properties
James. S. M. Anderson

The quantum theory of atoms in molecules (QTAIM) as originally formulated Prof. R.F.W. Bader and coworkers is a successful method for computing atomic properties within a nonrelativistic quantum mechanical framework. Prof. R.F.W. Bader and coworkers formulated a QTAIM that satisfies their treatment of Schwinger principle of stationary action for a volume and, as such, justifying its utility for computing atomic properties in a nonrelativistic setting. Relativity is critical when computing properties of chemical systems that include nuclei with atomic number larger than 37. It has been demonstrated how to formulate QTAIM to include relativistic effects in defining a proper quantum subsystem that satisfies Schwinger's principle of stationary action for the Scalar-Relativistic Zeroth-Order Regular Approximation (SR-ZORA) Hamiltonian. Given that the concept of an atom in a molecule is satisfied even when relativistic corrections are included a more practical question remains:
What level of theory is needed to obtain an accurate computation of a property?
Several properties at different levels of theory will be shown and provide intuition to properties that are sensitive to scalar-relativistic corrections, electron correlation, or both.

L-P1005
An Evaluation and Development of the Hybrid KS DFT Functionals Based on the KS Exchange-Correlation Potentials - the UMK26 hybrid functional.
Ireneusz Grabowski

We have developed a methodology for evaluating the quality of hybrid exchange-correlation (XC) density functional approximations (DFAs) based on fundamental quantities, i.e., Kohn−Sham (KS) XC potentials, self-consistent electron densities, first ionization potentials (IPs), and total energies. Since the XC potentials, the primary objects in the current study, are not directly accessible for the hybrids, we calculate them by inverting the KS electron densities. Using this methodology, we tested 155 hybrid DFAs from the LIBXC library, with FCI and CCSD(T) as reference methods. We have found that a group of functionals yields very good XC potentials, particularly those with a large mixture of Hartree−Fock exchange. Moreover, the value of IP strongly depends on the quality of the XC potential. Based on that, we show that the dominant qualitative features of correlation in hybrid DFAs do not arise primarily from the semilocal correlation functional itself, but instead from the difference between the semilocal exchange and exact-exchange contributions. This exchange-difference term is essential for restoring the physically correct structure of the correlation component of the exchange−correlation potential and the corresponding correlated density. In contrast, the semilocal correlation part acts mainly as a compensating contribution in the core and valence regions. Finally, we propose an interpretable construction principle for hybrid functionals in which the semilocal/exact-exchange difference is scaled in a controlled way. As a proof of concept, this methodology yields the simple global hybrid UMK26 functional.

L-P1006
Neuromorphic Devices Modulated by Quantum Effects and Ionic Coupling
Ya-Qian Liu

Brain-inspired neuromorphic devices that emulate integrated sensing–memory–computing are expected to overcome the von Neumann bottleneck. Quantum effects and ionic coupling can modulate carriers and excited states. This report introduces ion-gel-based biomimetic devices (tactile, auditory, and visual perception) and integrated sensing-memory-computing-display systems. It discusses quantum-confined emission, triplet excitons and intersystem crossing, trap-state storage, and ionic coupling regulation of synaptic plasticity. Their synergy can drive neuromorphic devices toward integrated sensing-memory-computing-display.

L-P1007
Multiphoton quantum plasmonic system
Mingyuan Hong

The quantum statistics of photons represent an important degree of freedom in multiphoton systems, yet their effective control has long remained challenging. This talk presents advances in multiphoton quantum plasmonics, from controlling photon statistics to exploring quantum statistical materials. Leveraging strong near-field coupling in a surface-plasmon platform, we demonstrate that nanostructures can modify photon statistics and use photon-number-resolving detection to resolve distinct multiphoton statistical subsystems. Building on these findings, we introduce the concept of quantum statistical metacrystals, in which engineered plasmonic structures create allowed and forbidden statistical bands, enabling statistical filtering and selective control of photon statistics. These studies highlight quantum statistics as a new degree of freedom for materials design, opening new avenues for statistical control, quantum imaging, and sensing.

L-P1008
Projection-Based DMRG-in-DFT Embedding for Strongly Correlated Molecular Systems
Libor Veis

Strongly correlated electronic systems remain among the most challenging targets of modern quantum chemistry, requiring methods capable of simultaneously describing static and dynamical electron correlation in increasingly large molecular systems. In this talk, I will present recent developments of projection-based density matrix renormalization group in density functional theory (DMRG-in-DFT) embedding methods for molecules with strongly correlated fragments. The projection-based embedding framework combines the accuracy of wave function methods for an active subsystem with the computational efficiency of density functional theory for the environment, enabling applications to chemically relevant systems beyond the reach of conventional multireference approaches. I will first introduce the original DMRG-in-DFT formulation and demonstrate its performance for prototypical strongly correlated problems, including bond dissociation and transition-metal complexes. Next, I will discuss recent advances aimed at improving the accuracy of the coupling between the active subsystem and its environment. In particular, I will show how errors originating from approximate nonadditive exchange-correlation contributions can be substantially reduced by combining exact exchange with multireference adiabatic connection corrections to the nonadditive correlation energy. Applications to dissociating systems demonstrate significant improvements over conventional embedding approaches. Finally, I will present the formal theoretical foundations of projection-based wave function-in-DFT embedding and discuss why the conventional projection-based formulation cannot be exact even in the limit of the exact exchange-correlation functional. This analysis identifies the fundamental sources of embedding errors in strongly correlated systems and clarifies the role of nonadditive exchange-correlation effects at the subsystem interface.

L-P1009
Investigation of medium-sized methane clusters with quantum chemical first principles and ab initio calculations
Michael Dolg

The incremental scheme was originally devised by H. Stoll in the 1990ies to obtain wavefunction-based ab initio calculations for correlation energies per unit cell of crystalline solids, e.g. CCSD or CCSD(T) energies for diamond or graphite. Due to the relatively small number of contributing energy increments for simple/small unit cells the calculations could be essentially carried out in a non-automated way. For general larger molecules this procedure becomes impracticable due to the lack of symmetry. Three previous implementations of the approach for corresponding fully automated calculations on medium-sized and large molecules will be briefly reviewed and a new variant especially optimized for molecular clusters and potentially linear scaling for large systems is reported. As an application structures, stabilities and vibrational frequencies of methane clusters with 10 to 40 monomers have been derived at the B3LYP+D3+BJ def-TZVPP level. Single-point incremental CCSD(T)-F12 VTZ-F12 calculations up to 3rd order (with up to 4000 contracted basis functions) as well as corresponding rigid monomer geometry optimizations were performed with the new approach and reveal that the B3LYP+D3+BJ def-TZVPP

structures and energies are quite accurate. A necessary specialized explicit treatment of low-energy inter-monomer vibrations and (hindered) monomer rotations as well as the influence of nuclear spin states is discussed. Finally, using corresponding values for the cluster heat of formation the heat of vaporisation of methane at the boiling point 111 K is estimated by extrapolation to be about 7 kJ/mol (exp. 8.19 kJ/mol).

L-P1010
Superadiabatic engineering of quantum state transfer across multi-state platforms
Jin-Lei Wu

Superadiabatic (SUAD) driving provides a powerful shortcut to adiabaticity, enabling fast and high-fidelity quantum state engineering across multi-state systems. We demonstrate this paradigm in three distinct platforms. On photonic chips, we realize SUAD topological pumping via gap-mode engineering, achieving a 20-fold footprint reduction over conventional adiabatic schemes. In superconducting transmon qudits, we design modified SUAD pulse envelopes for multiphoton LZSM transitions, accelerating two- and three-photon population transfers by factors of four and three, respectively, with near-unity fidelity and enhanced decoherence resilience. In two interacting Rydberg atoms, we apply SUAD to the two-photon LZSM process, reducing operation time by 67% and infidelity by 68% under realistic decoherence. Across all platforms, our protocol modifies only the envelope of the existing drive field without introducing auxiliary controls. These results establish SUAD as a versatile, experimentally friendly framework for accelerated quantum state transfer in multi-state systems, with direct applications in quantum photonics, superconducting circuits, neutral-atom arrays, and scalable hybrid quantum networks.

L-P1011
Liquid photonic-molecule microlasers for ultrasensitive biosensing
Yan Wang

Droplet microlasers, as promising tools for biophotonics and biomedical sciences, have witnessed rapid advances due to their flexible reconfigurability, high sensitivity to stimuli, and label-free biosensing capability. However, designing these biosensors with the simultaneous advantages of a low lasing threshold, high spectral purity, and ultrahigh sensitivity remains challenging. Here, we propose a versatile strategy for constructing liquid photonic molecules (LPMs) that integrate these features within a single device. By tailoring the spectral Vernier overlap in size-mismatched droplets, the device enables single-mode lasing with a low threshold of approximately 610 nJ $mm^{-}2$. The LPM lasers are further engineered for dynamic tunability through a molecular isomerization strategy, which induces spectral mode hopping and yields nearly a tenfold enhancement in spectral sensitivity compared with single droplets. Moreover, by leveraging the self-referenced intensity response of the LPM lasing modes, we demonstrate a three-orders-of-magnitude enhancement in biomolecular sensing, achieving a detection limit of 30 aM and a dynamic range spanning nine orders of magnitude. Our work provides a promising platform for bio-integrated liquid sensors and related biophotonic applications.

L-P1012
Optical coherent control of biological electron transfer
Dongping Zhong

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.

L-P2001
Fluxional Covalent Bonds, Hydrogen Bonds, and Halogen Bonds in Chemistry
Si-Dian Li

Bonding is the nature of chemistry which determines the structures and properties of molecules and materials. Chemical bonds form and break constantly under certain conditions. Based on extensive first-principles theory calculations, BOMD simulations, and AdNDP and QTAIM bonding analyses on a series of experimentally known clusters, molecules, and crystals, our group proposed the concept of fluxional bonds (**FBs**) in chemistry as an extension of the classical localized and delocalized bonds in the area, unveiling the fluxional bonding nature of structural fluctuations. We mainly focus in this work on (**1**) Fluxional covalent bonds (**FCBs**) in planar B_{11}^-, B_{13}^+, and B_{19}^- (**Fig.1a**), tubular $Ta@B_{20}^-$, and cage-like B_{40} and B_{39}^-; (**2**) **FCBs** in bullvalene $C_{10}H_{10,}$ semibullvalene C_8H_8, and their analogs; (**3**) Fluxional hydrogen bonds (**FHBs**) in small water clusters $(H_2O)_n$ (n=2-6) (**Fig.1b**) and boric acid clusters $(B(OH)_3)_n$ (n=2-6); and (**4**) Fluxional halogen bonds (**FXBs**) in the twinned co-crystal (1β+1β') of 1,4-diiodobenzene and 1,4-dinitrobenzene at low temperatures (<130 K). The corresponding fluxional rate constants k_{TST} have also been calculated to facilitate the future experimental characterization of FBs in chemistry.

L-P2002
Ultrafast charge migration: simulations, manipulations, and applications
Yonggang Yang

Quantum science and technology call for coherent quantum processes. Decoherence is an inevitable enemy. Decoherence may be followed, however, by a friend: (partial) recoherences. Our example is charge migration in small molecules. It may be initiated by an ultrashort laser pulse which generates a superposition of electronic states. If the nuclear wave functions in different electronic states run away from each other, their overlap decays, and this causes decoherence of charge migration, on typical time scales of few fs. Nuclear motions may, however, cause (partial) revivals of the overlaps. As a consequence, this induces recoherences of charge migration. The phenomenon is demonstrated by quantum dynamics simulations of the concerted time evolutions of the nuclear and electronic densities in several molecules. The dependence of the coherences on the size of molecules are investigated. We further performed manipulations of the coherences of charge migration with laser pulses. Among various types of charge migrations there is one peculiar motions of electrons along a three dimensional helical path. They can be launched by two circularly polarized laser pulses. Detailed and extended investigations on this type of charge migration shows that such two circularly polarized laser pulses can generate electronic chirality in pre-oriented achiral molecules. The electronic chirality may flip on times scales from femtosecond to attosecond.

L-P2003
Photonic spin Hall effect: Manipulations and applications
Xinxing Zhou

The photonic spin Hall effect (SHE) manifests itself as the spin-dependent splitting of left- and right-handed circularly polarized components when a linearly polarized light beam is reflected or refracted from the media interface. The physical mechanism of this phenomenon is due to spin-orbit interaction of light. Until now, the photonic SHE has been widely investigated in different physical systems such as optical interfaces, metasurfaces/metamaterials, near-field optics, topological and disordered systems, as well as non-Hermitian photonics. Significantly, the photonic SHE provides the unique spin degrees of freedom to flexibly control light, which has enabled tremendous applications in precise metrology, spin-based nanophotonic devices, and mathematical operations. In this talk, we will introduce our recent works about manipulations and applications of photonic SHE.

L-P2004

Quantum-Interference Control of Single-Photon Transport and Frequency Conversion in Waveguide QED

Ya-Ju Song

Quantum interference provides an important mechanism for controlling single-photon dynamics in waveguide quantum electrodynamics. In this talk, I will present some recent work on coherent single-photon transport in structured waveguides. For multilevel emitters coupled to rectangular waveguides, we investigate how atomic interference and transverse-mode effects influence photon transmission and reflection, with particular attention to the multi-mode regime. We further consider a coherently driven three-level emitter and show how an external field can provide additional control over single-photon scattering, including its dependence on the photonic input state. Finally, I will briefly discuss an extension to giant-atom waveguide systems, where spatially separated coupling points offer additional degrees of freedom for manipulating photon propagation and frequency conversion. These results illustrate how different interference mechanisms can be used to control single-photon transport in waveguide QED.g

L-P2005

Recent developments of density-matrix based quantum embedding approaches to strongly correlated systems

Hong Jiang

Developing electronic structure theory for strongly correlated systems (SCSs) is regarded as one of the greatest challenges in molecular quantum chemistry and condensed matter theory. A lot of efforts have been devoted to the development of various quantum embedding theory techniques to treat complex SCSs accurately and efficiently. Density-matrix embedding theory (DMET), formulated based on the Schmidt decomposition of Slater determinants, provides a systematic framework to combine low- and high-level quantum chemistry methods to treat strongly correlated systems. In this lecture, I will give a brief overview of quantum embedding theory and present our recent efforts of further developing and applying DMET-based quantum embedding approaches to strongly correlated systems including 3d and 4f single-ion magnets (SIMs) and lanthanide luminescent complexes.

L-P2006

M-The Density Knows: Information-Theoretic Learning from Molecular Response to Multiproperty Prediction

Dongbo Zhao

Accurate prediction of molecular properties must balance quantum-mechanical accuracy with computational efficiency, scalability, transferability, and physical interpretability. This presentation introduces a density-centered framework that combines information-theoretic approach (ITA) descriptors, generalized energy-based fragmentation (GEBF), and machine learning to predict molecular response and physicochemical properties across molecular, macromolecular, and condensed-phase systems. Starting from the ground-state electron density, quantities derived from Shannon entropy, Fisher information, and others provide compact and physically motivated representations of electronic structure. Linear relationships between these descriptors and molecular polarizability were first established for amino acids and peptides and subsequently transferred, through GEBF, to proteins whose full-system wave functions are computationally inaccessible. Extension to periodic boundary conditions enabled efficient prediction of post-Hartree–Fock polarizabilities for condensed-phase systems. Remarkably, cheap Hartree–Fock densities could encode sufficient information to reproduce correlated response properties for systems containing hundreds to more than one thousand atoms. Replacing linear regression with deep learning further enabled the simultaneous prediction of polarizabilities and NMR shieldings for proteins and protein aggregates exceeding 4000 atoms. The same family of density-based descriptors was then generalized beyond response properties to electron-correlation energies, redox potentials, octanol–water partition coefficients, and excitation energies. Together, these studies trace a coherent progression from density–property relationships to scalable and multiproperty learning. Electron density supplies the common physical representation, fragmentation provides access to large systems, and deep learning captures nonlinear mappings between electronic structure and diverse observables. This framework offers a physically grounded alternative to purely structure-based black-box models and provides a route toward transferable, interpretable, and closed-loop molecular property prediction.

L-P2007

Synthetic Chemistry of Porphyrinoids

Jianxin Song

Control electronic or excitonic interactions or manipulation electronic current in conjugated pi-system are important and difficult, and which is a key step to produce new materials. How to construction of Porphyrin arrays and preparation of new porphyrinoids efficiently are very important in porphyrin chemistry. Usually, unique structure comes out with special properties. Porphyrinoids have been extensively explored as synthetic models of photosynthetic antenna and functional hosts possing convergent multi-dentate coordination sites. Multipyrrolic macrocycles with the change of the meso carbon and pyrrole unit exhibit different structures and fascinating properties. Highly conjugated multi-porphyrin arrays have received much attention in light of their potential applications in optoelectronic devices, sensors, photovoltaic devices, non-linear optical (NLO) materials, photodynamic therapy (PDT) pigments, and light-harvesting models. The manipulation of interporphyrinic interaction is often essential to achieve desirable electronic and photophysical properties. Palladium catalyzed cross coupling of borylated porphyrins and aryl halides, it is widely used to synthesize some porphyrin arrays which could not be obtained in other strategies. We have successfully synthesized 2,5-thienylene/pyrrolyene bridged β-to-β porphyrin nanorings, 2,6-pyridylene-bridged β-to-β porphyrin nanorings, β-to-β terpyridylene/azobenzene bridged porphyrin nanorings, meso-to-meso azobenzene/2,5-pyrrolyene bridged porphyrin nanorings, directly Pd(II) -bridged porphyrin belts, porphyrin barrel, and meso,meso-porphyrinic bridged β-to-β porphyrin nanorings by this way, and β-to-β spacer-free porphyrin arrays were also constructed recently in our lab. Although the borylated porphyrins are almost able to react with any aryl halides bought from market, we found it is difficult to synthesis some elegant porphyrin arrays. How to increase the dissolubility and prepare the building blocks are challenges for construction of elagant multiporphyrin arrays. Some new porphyrin arrays recently have been synthesized through Pd-catalyzed cross-coupling reactions or aldehyde condensation and oxidation in our group with suitable precusor. Some new porphyrinoids have also been explored including earring porphyrins and smaragdyrins. Smargdyrin is a historic and puzzling molecule, as its discovery was reported along with sapphyrin by Woodward early in 1966, but its synthesis has not been accomplished so far. Our group reported the first synthesis of earring porphyrins and meso-trimesityl [20]smaragdyrin as a stable antiaromatic compound under ambient conditions. Our synthetic strategy involves a double SNAr reaction of 1,9-dibromo-5-mesityldipyrrin 1 with 5,10-dimesityltripyrran 2 as a key step. Both precursors 1 and 2 were prepared according to the reported methods from our group. After extensive experimentations, we found that refluxing of an equimolar mixture of 1 and 2 in p-xylene in the presence of Cs2CO3 for 48 h gave [22]smaragdrin BF2 complex 3 in 13% yield. To the best of our knowledge, this is the first example of the synthesis of expanded porphyrins by SNAr reaction of tripyrrane anion. Antiaromatic compound 5 is very stable but aromatic compound 6 is easy to be oxidated in air. Neo-confused smaragdyrin were also synthesized in good yield.

L-P2008

Synthesis, Structure, and Properties of π-Extended Porphyrinoids

Kaisheng Wang

Porphyrinoids play an important role in dye-sensitized solar cells, nonlinear optical devices, and photodynamic therapy. However, to address the lack of efficient construction strategies for π-extended porphyrinoids, we have recently synthesized a series of novel π-extended porphyrinoids: (1) polycyclic aromatic hydrocarbons (PAHs)-fused porphyrins; (2) triply linked porphyrin/anthracene-norcorrole hybrids; (3) BODIPY-embedded antiaromatic nanographenes. The correlations between different fused moieties and molecular ground-state electronic structures, together with their photophysical and electrochemical properties, were systematically investigated. Theoretical foundations and experimental support derived from these studies provide a basis for the design of porphyrin-based functional molecules, thereby offering new insights into metal-free magnets, organic semiconductors, and near-infrared dyes.

L-P2009
Chemistry of Subporphyrin Borenium cations
Ling Xu

Since the first synthesis in 2006, subporphyrin has received considerable attention as the smallest contracted porphyrin. Neutral subporphyrins exhibit bowl-shaped conformations, whereas subporphyrin borenium cations display planar structures. When the subporphyrin borenium cations are forced to adopt bowl-shaped conformation, the vacant p orbital of the central boron become highly exposed, thereby displaying enhanced acidity and enabling them to act as super Lewis acids.
The triply-linked subporphyrin dimer was utilized as the model compound, in which both subporphyrin subunits adopt highly constrained bowl-shaped conformation. Oxidation of the dimer with Ag+ affords the corresponding cation radical and dication species. The following axial C-B bond cleavage upon heating furnishes the bowl-shaped subporphyrin borenium cation, which immediately abstracts a fluoride ion from SbF6- to form an axial B-F bond.

L-P2010
Site-selectivity-enabled novel fused porphyrins: precise synthesis and property investigation
Mingbo Zhou

Porphyrin-based molecules play a significant role in high-performance materials, artificial photosynthesis, biomimetic catalysis, and photodynamic therapy. Design and synthesis of structurally diverse porphyrins while uncovering the structure-properties relationship are not only central research of porphyrin chemistry but also pave the way for innovative solutions in energy, healthcare, and environmental fields. By integration of substrates design with post-synthetic modifications strategy, we have recently synthesized a series of pyrrole-sharing fused porphyrinoid hybrids and novel porphyrin oligomers in which the resulting six- to eight-membered-heterocycles are served as fused bridges[1-6]. Moreover, their structure-properties relationship gains a deeper understanding. These studies provide both theoretical foundations and experimental support for the development of porphyrin-based functional molecules, therefore offering new insight for research in high-performance materials, coordination chemistry, catalysis, and related fields.

L-P3001
Quantum Multiparameter Estimation and Imaging: Fundamental Limits, Measurement Incompatibility, and Resolution Enhancement
Xiao-Ming Lu

Quantum multiparameter estimation provides a general framework for estimating several parameters simultaneously, but its ultimate precision is constrained by fundamental limits and by measurement incompatibility. In this talk, we investigate these fundamental limits and analyze how incompatible measurements affect the attainable estimation precision. We further apply quantum multiparameter estimation to the problem of imaging resolution, offering a quantum-information perspective on resolution limits. In particular, we discuss spatial mode demultiplexing as a strategy to improve imaging resolution. Our study connects quantum estimation theory with practical imaging, highlighting both fundamental constraints and opportunities for resolution enhancement.

L-P3002
Quantum Control of Ultracold Molecules: From Quantum States to Quantum Gates
Chuancun Shu

In this talk, Prof. Chuancun Shu will present recent advances in quantum control of molecular systems, from two-level qubits to multi-level qudits. He will first give an overview of quantum control in molecular qubits, highlighting challenges from the complex rotational and vibrational structures of polar molecules. He will then present his group's key contributions to analytical methods for solving wave functions and time-evolution operators in multi-level quantum systems. These methods enable precise mapping between coherent superpositions of molecular states and microwave pulse sequences, allowing accurate quantum-state manipulation. He will also cover systematic designs of composite microwave pulse sequences for universal quantum gates—single-qubit, qutrit, and general qudit—with improved robustness against systematic errors. These advances enable scalable molecular quantum processors exploiting the rich Hilbert space of rotational states, with applications in quantum simulation, metrology, and quantum information science.

L-P3003
Spin Effects and Spin Control in Hybrid Semiconductors
Yaxin Zhai

Organic–inorganic hybrid semiconductors combine the highly tunable nature of organic components with the excellent optoelectronic properties of inorganic semiconductors, providing a unique materials platform for the generation, transport, and manipulation of spin degrees of freedom. This presentation will first introduce the fundamental concepts of spintronics in hybrid semiconductors and the principal experimental approaches for investigating spin dynamics. It will then focus on three representative spin-related phenomena in these systems: the chiral-induced spin selectivity (CISS) effect, spin funneling, and the Rashba effect, with particular emphasis on their distinct physical origins and roles in spin generation, transport, and manipulation. Finally, I will discuss emerging physical processes arising from the coexistence and synergistic interplay of multiple spin effects within the same material or heterostructure, and explore the potential for achieving efficient and multidimensional spin control by exploiting the complementary functionalities of different spin mechanisms.

L-P3004
Universal scaling behavior in topological quantum phase transitions under driven critical dynamics
Fuxiang Li

The Kibble-Zurek mechanism (KZM) is a central theory in nonequilibrium statistical physics, originally proposed to explain topological defect formation in the early universe and later extended to continuous phase transitions in condensed matter systems. It describes the nonequilibrium dynamics of systems driven through phase transitions, especially the universal scaling of defect density with quench rate. We systematically study defect characterization and novel universal scaling behavior in topological quantum phase transitions under driven critical dynamics. By

analyzing the driven dynamics of bulk and boundary order parameters at topologically distinct quantum critical points (QCPs) in quantum spin chains, and by studying defect production in free-fermion models, we show that topological edge modes at criticality give rise to anomalous dynamical scaling. While the bulk dynamics remain indistinguishable and follow standard Kibble-Zurek scaling, the boundary dynamics exhibit anomalous scaling unique to topological criticality, obeying modified scaling relations beyond the traditional KZ framework. We further find that in higher-order topological phase transitions, the conventional KZM breaks down and anomalous scaling exponents emerge. For two-dimensional boundary-obstructed higher-order topological systems, the KZ scaling must be modified to accommodate the effective dimension of the topological edge bands rather than the actual physical dimension; boundary conditions also significantly affect the scaling behavior. These findings reveal new physical phenomena arising from the interplay between topology and nonadiabatic dynamics, and enrich our understanding of defect-generation mechanisms in nonequilibrium processes.

L-P3005

Magnetoelectric Coupling and Quantum Transport in Two-Dimensional Compensated Magnets

Jian-Sheng Dong

Two-dimensional compensated magnets, characterized by vanishing net magnetization, robust magnetic order, and intertwined spin, valley, layer, and ferroelectric degrees of freedom, provide a versatile platform for low-power, nonvolatile control of quantum states and emergent quantum transport phenomena. This talk presents our recent theoretical studies on magnetoelectric coupling and quantum transport in two-dimensional antiferromagnets and altermagnets, with a focus on sliding ferroelectric antiferromagnets, altermagnetic bilayers, and fractional quantum ferroelectric altermagnets. In bilayer VS2, a sliding ferroelectric antiferromagnet, interlayer sliding induces an out-of-plane ferroelectric polarization, while both ferroelectric polarization reversal and magnetic-order reversal can reconstruct the spin, valley, and layer degrees of freedom, enabling dual electric and magnetic control of a layer-locked anomalous valley Hall effect. In altermagnetic bilayer Fe2WS4, the sliding direction acts as an internal symmetry-selective control parameter. Diagonal sliding induces ferroelectric polarization reversal and switches the momentum-space spin texture and anomalous Hall response, whereas axial sliding lifts the degeneracy between the X and Y valleys, giving rise to reversible valley polarization and a switchable anomalous valley Hall effect. In monolayer Cr2S2, a fractional quantum ferroelectric altermagnet, fractional quantum ferroelectric switching reverses the altermagnetic spin splitting, interchanges the spin characters of the X and Y valleys, and reconstructs the Berry-curvature distribution without rotating the Néel vector, thereby realizing polarization-controlled spin-valley locking and valley Hall effects. In addition, related fractional quantum ferroelectric systems will be discussed to illustrate how strain and structural asymmetry can further modulate valley, spin, and transport responses. These studies establish ferroelectric polarization, interlayer sliding, and fractional quantum ferroelectric switching as effective routes for controlling magnetoelectric coupling, coupled quantum degrees of freedom, and Berry-curvature-driven transport in two-dimensional compensated magnets, offering new insights into multistate quantum devices and low-power spin-valleytronic applications.

L-P3006

Reinforcement-learning-assisted nonreciprocal optomechanical gyroscope

Qing-Shou Tan

We propose an optomechanical gyroscope architecture based on a spinning cavity optomechanical resonator evanescently coupled to a tapered optical fiber without relying on costly quantum light sources. Our study reveals a striking dependence of the gyroscope's sensitivity on the propagation direction of the driving optical field, manifesting robust quantum nonreciprocal behavior. This nonreciprocity significantly enhances the precision of the angular-velocity estimation, offering a unique advantage over conventional gyroscopic systems. Furthermore, we demonstrate that the operational range of this nonreciprocal gyroscope is fundamentally governed by the frequency of the pumping optical field, enabling localized sensitivity to angular velocity. Leveraging the adaptive capabilities of reinforcement learning (RL), we optimize the gyroscope's sensitivity within a targeted angular velocity range, achieving unprecedented levels of precision. These results highlight the transformative potential of RL in advancing high-resolution, miniaturized optomechanical gyroscopes, opening new avenues for next generation inertial sensing technologies.

L-P3007
Memory kernel coupling theory to quantum dynamics
Wenjie Dou

Time correlation functions (TCFs) are fundamental quantities governing transport coefficients, optical spectra, and chemical reaction rates. However, accurately calculating TCFs for complex quantum systems remains a major computational challenge because conventional approaches generally require propagating the full quantum dynamics. We developed Memory Kernel Coupling Theory (MKCT), a new framework for directly computing time correlation functions from higher-order moments. Rather than explicitly propagating projected dynamics, MKCT decomposes the memory kernel into a hierarchy of auxiliary kernels governed by linearly coupled equations. This formulation requires only a single steady-state calculation, making the computational cost largely independent of system size. Benchmark on both bosonic and fermionic open quantum systems demonstrate that MKCT reproduces numerically exact results. Because MKCT is not restricted to Gaussian environments or linear system-bath couplings, it establishes a broadly applicable framework for studying quantum dynamics in realistic systems.

L-P3008
Electrically tunable non-Hermitian magnon propagation in magnetic waveguides
Xi-guang Wang

Spin waves arise from the collective precession of magnetic moments in magnetic materials, and their quanta — magnons — exhibit unique physical properties that make them ideal information carriers for building next-generation, higher-performance information devices. Realizing such magnonic information devices requires efficient control over magnon transport properties. For this purpose, we propose using current-induced spin-orbit torque to drive spatial variations in magnon gain and loss — an approach that gives rise to a range of non-Hermitian phenomena, including PT-symmetric magnons and their associated phase transition, Floquet engineering of non-Hermitian magnons, unidirectional invisible magnon transport, magnon bound states in the continuum, and magnon lasing/anti-lasing, thereby enabling efficient generation and control of non-Hermitian magnons. These results provide a new route for the electrical control of magnon propagation and a new strategy for realizing low-power magnonic components.

L-P3009
Robust Quantum Control and Sensing in Defect Spin Systems
Qiong Chen

High-sensitivity quantum sensing requires both reliable state manipulation and the preservation of target-signal responses during coherence protection. However, control-field inhomogeneities and environmental noise degrade gate fidelity, while intrinsic system couplings can suppress the linear response to weak signals. Addressing these challenges, this presentation outlines dynamic control protocols tailored for solid-state defect spin systems. By exploiting energy-level structures and geometric adiabatic evolution, we decouple state inversion from microwave amplitude fluctuations, realizing robust spin control and efficient nuclear spin hyperpolarization. Furthermore, through periodic driving modulation and Hamiltonian engineering, we circumvent the non-commutative suppression induced by intrinsic transverse coupling, mitigating environmental noise while restoring the linear signal response for high-frequency AC field detection. These methodologies provide practical solutions for high-fidelity spin manipulation in complex environments and open new avenues for broadening the scope of precision quantum sensing.

L-P3010

Experimental witness of quantum jump induced high-order Liouvillian exceptional points

Jian-Qi Zhang

The exceptional point has presented considerably interesting and counterintuitive phenomena associated with nonreciprocity, precision measurement, and topological dynamics. The Liouvillian exceptional point (LEP), involving the interplay of energy loss and decoherence inherently relevant to quantum jumps, has recently drawn much attention due to capability to fully capture quantum system dynamics and naturally facilitate non-Hermitian quantum investigations. It was also predicted that quantum jumps could give rise to third-order LEPs in two-level quantum systems for its high dimensional Liouvillian superoperator, which, however, has never been experimentally confirmed until now. Here we report the observation of the third-order LEPs emerging from quantum jumps in an ultracold two-level trapped-ion system. Moreover, by combining decay with dephasing processes, we present the experimental exploration of LEPs involving combinatorial effect of decay and dephasing. In particular, due to non-commutativity between the Lindblad superoperators governing LEPs for decay and dephasing, we witness the movement of LEPs driven by the competition between decay and dephasing occurring in an open quantum system. This unique feature of non-Hermitian quantum systems paves a new avenue for modifying nonreciprocity, enhancing precision measurement, and manipulating topological dynamics by tuning the LEPs.

L-P3011

Friedel oscillations in semi-Dirac and altermagnet systems

Xiao-Ying Zhou

We present a theoretical study comparing the power-law decay behavior of Local Density of States (LDOS) oscillations near a line defect in two distinct anisotropic two-dimensional electron systems: systems featuring Semi-Dirac (SD) points and monolayer Black Phosphorus (BP). Utilizing a low-energy k·p Hamiltonian and the stationary phase approximation, we analytically derive the LDOS decay indices (α) to characterize the long-range electronic response. For SD point systems, the decay is strongly anisotropic: the index is a unique −5/4 when the line defect is perpendicular to the linear dispersion direction (becoming −1/4 if gapped), but reverts to a conventional −1/2 when perpendicular to the parabolic dispersion direction. This −5/4 index provides a distinctive fingerprint for identifying the semi-Dirac phase. In contrast, for monolayer Black Phosphorus, whose properties are known to be highly anisotropic, the power-law decay index exhibits a remarkable isotropic behavior, always equaling −1/2 regardless of the defect's orientation. This −1/2 index aligns with that of a conventional 2D semimetal, although the magnitude and period of the LDOS oscillations remain highly sensitive to the defect's angle, reflecting BP's inherent anisotropy. Our results demonstrate that the LDOS decay index is a critical feature for distinguishing between different types of anisotropic band structures and serves as an experimentally accessible signature using techniques like Scanning Tunneling Microscopy (STM).

L-P4001
Dark Mode and Dark State Theory in Quantum Physics
Jie-Qiao Liao

Dark mode and dark state effects are novel physical phenomena in quantum systems caused by destructive quantum interference. They not only have important academic value in the fundamental research of quantum theory, but also provide broad application prospects for the development of modern quantum technology. Dark mode and dark state effects play a dual role in quantum technology applications. On the one hand, they can be used to achieve adiabatic quantum state transfer; On the other hand, they also suppress the transfer of quantum resources between bright and dark modes/states. Therefore, building accurate methods for determining dark mode and dark state effects in quantum systems, and developing effective control measures for dark mode and dark state effects, have become key issues that urgently need to be addressed in quantum physics and quantum optics. This talk focuses on the coupled bosonic networks and coupled light-atom systems, systematically elaborating on the physical origins, basic characteristics, determination theorems, and control methods of dark mode and dark state effects, and delving into their potential application value and development prospects in quantum information science.

L-P4002
Tensor-Network Machine Learning: Trainability, Generalization, and Statistical Structure
Liwei Yu

Tensor networks offer a structured framework for quantum-inspired machine learning that incorporates locality, geometry, and entanglement. Yet the trainability, generalization, and statistical behavior of tensor-network models remain incompletely understood. In this talk, I present three theoretical results. First, I show how the choice between global and local loss functions affects the emergence of barren plateaus. Second, I discuss no-free-lunch bounds for tensor-network learning and their connection to adversarial vulnerability. Third, I examine when tensor-network models exhibit Gaussian-process behavior and when non-Gaussian behavior persists under different scaling regimes. Together, these results clarify the capabilities and fundamental limitations of tensor-network machine learning.

L-P4003
A Unified Framework for Sequential Quantum Correlation Sharing
Changliang Ren

Quantum measurements not only extract information but also reshape quantum states through measurement backaction, thereby determining how quantum resources can be distributed and recycled. In this talk, recent progress on the sequential sharing of quantum correlations will be reviewed from the perspective of generalized quantum measurements and quantum instruments. Particular emphasis will be placed on Bell nonlocality, EPR steering, entanglement, network nonlocality, and contextuality under sequential and weak-measurement scenarios. Recent advances on complementarity-based correlation sharing and unified measurement frameworks beyond conventional POVM descriptions will also be discussed, highlighting how different Kraus structures govern resource dissipation, robustness, and quantum resource recycling in multipartite and sequential quantum information protocols.

L-P4004
Nonreciprocal and non-Hermitian photon blockade effects
Ran Huang

Photon blockade (PB) provides a fundamental mechanism for generating nonclassical light at the single- or few-photon level and constitutes an important building block for quantum photonic technologies. Conventional PB, however, is typically reciprocal and often relies on stringent conditions on optical nonlinearity, dissipation, and system parameters, posing challenges for directional operation, active control, and robustness. In this talk, I will present our recent efforts toward engineering PB through nonreciprocity, non-Hermiticity, and ultrastrong light–matter interactions. I will first introduce nonreciprocal PB, where the quantum statistics of light become direction dependent, enabling fundamentally different photon transport behaviors for opposite propagation directions. I will then discuss how non-Hermitian physics, including loss engineering and chiral exceptional points, provides additional degrees of freedom for suppressing, reviving, and switching PB. These concepts further motivate strategies for improving the robustness of single-PB against parameter variations and realistic imperfections. Finally, I will discuss recent extensions toward hybrid molecular optomechanical systems and the ultrastrong-coupling regime, where unconventional light–matter interactions enable robust PB and few-polariton quantum effects. Together, these studies illustrate how nonreciprocity, non-Hermiticity, and engineered light–matter interactions can transform PB from a conventional nonlinear quantum-optical effect into a versatile platform for controlling quantum light, with potential applications in single-photon devices, quantum information processing, and integrated quantum photonics.

L-P4005
Machine-learning-assisted quantum state engineering in cavity optomechanical systems
Yu-Hong Liu

We investigate machine-learning-assisted optimization of optical driving for quantum state engineering in cavity optomechanical systems. Two representative parameter regimes are considered: the strongly driven linearized regime and the single-photon strong-coupling regime. In the linearized regime, we construct an optimization model based on linear Gaussian quantum dynamics, combining gradient descent with neural network mappings. The optimized optical drives enable ground-state cooling beyond the sideband-cooling limit for a single cavity under continuous-wave driving in the strong-coupling regime. They also enhance optomechanical entanglement to two to three times its steady-state value and achieve mechanical squeezing beyond the 3 dB limit. In the single-photon strong-coupling regime, we develop a reinforcement learning optimization model based on a dressed-state master equation. The model employs the twin delayed deep deterministic policy gradient algorithm to optimize optical driving. This approach enables high-fidelity deterministic preparation of mechanical Fock states, superpositions of Fock states, and entangled states of two oscillators. These results demonstrate that machine learning provides an effective approach to optimizing complex optical drives in cavity optomechanical systems. They also offer new perspectives on related quantum control problems.

L-P4006
Multi-Parameter Quantum Positioning Schemes for Different Scenarios
Yong-Qiang Li

Quantum positioning, as an important research direction in quantum sensing and quantum information science, holds significant promise for surpassing the precision limits of classical measurements and enhancing target sensing capabilities in complex environments. For complex target positioning tasks, joint multi-parameter estimation, high-precision measurement, and measurement stability constitute three key scientific challenges in the development of high-performance quantum positioning. In recent years, nonclassical resources, such as quantum entanglement and quantum interference, have provided new approaches for efficiently extracting multi-parameter information from complex targets and achieving high-precision measurements.
This report focuses on our group's recent research on quantum positioning of complex targets. In particular, we will present a multi-target, multi-parameter joint estimation method based on two-photon entangled sources, a two-dimensional high-precision quantum positioning scheme based on two-mode squeezed entanglement, and a highly stable three-dimensional quantum positioning scheme based on Hong–Ou–Mandel (HOM) interference and polarization control.

These approaches are designed to enable the joint estimation of multiple parameters associated with complex targets. Under appropriate measurement conditions, they can achieve the quantum precision limit while effectively mitigating fluctuations in positioning precision arising from the parameter dependence of the quantum Fisher information. These results provide new approaches for realizing high-precision and highly stable quantum positioning in complex scenarios.

L-P4007
Temperature-enhanced quantum sensing
Ji-Bin Yuan

We study a dephasing qubit as a probe of its environment. We show that raising the temperature can enhance, rather than degrade, the achievable precision. Precision is quantified by the quantum Fisher information and the dimensionless quantum signal-to-noise ratio. Two settings are considered.
In the first setting, an impurity qubit is immersed in a quasi-two-dimensional dipolar Bose–Einstein condensate, whose collective excitations act as a dephasing reservoir. We estimate the relative dipole–dipole interaction strength. Roton softening renders the dephasing strongly non-Markovian, so that the quantum Fisher information grows with encoding time. Raising the temperature further accelerates this growth: the concurrent enhancement of the sensitivity of the decoherence factor to the parameter outweighs the loss of probe coherence.
In the second setting, a single dephasing qubit estimates the cutoff frequency of Ohmic-family environments, characterized by the coupling strength, the Ohmicity parameter, and the cutoff frequency. Increasing the scaled temperature shortens the optimal measurement time and raises the optimal quantum signal-to-noise ratio, by nearly two orders of magnitude for certain Ohmic-family environments.
In both settings, temperature serves as a resource for enhancing the precision of quantum sensing.

L-P4008
Advanced quantum metrology with Hong-Ou-Mandel interferometers
Rui-Bo Jin

We present our recent three works on Hong-Ou-Mandel (HOM) interferometer-based quantum measurements: Firstly, we propose and experimentally demonstrate a sample-half-inserted HOM (SHOM) interferometer, which enhance the Fisher information by 5 orders of magnitude in a single interference event. Secondly, we show spectral characterization of biphotons using quantum interferometric spectroscopy. Finally, we show 4780 nm ultra-broadband entangled biphotons from a chirped PPLN, which can realize a 965-attosecond-wide HOM dip.

L-P4009
Hybrid Cavity Optomechanics: A Versatile Platform for Manipulating Macroscopic Quantum Entanglement
Yafeng Jiao

Quantum entanglement is a unique property of quantum mechanics, which plays an important role in both fundamental quantum science and emerging quantum technologies. However, quantum entanglement always tends to be destroyed by non-ideal factors in open quantum systems. Hybrid cavity optomechanical systems offer an ideal platform for exploring macroscopic quantum coherence due to their exceptional tunability and versatile interface with diverse quantum architectures. In this talk, we present how to integrate various quantum subsystems to leverage their unique quantum advantages, and discuss methods to generate, manipulate, safeguard, and detect bipartite and multipartite entanglement within hybrid optomechanical platforms.

L-P4010
New Developments and Applications of Relativistic Energy-consistent Pseudopotentials
Xiaoyan Cao

New energy-consistent relativistic Ln f-in-valence pseudopotentials are presented and test calculations for CeO are reported. Related f-in-core and f-in-valence An pseudopotentials were applied in first-principles (BP86) and ab initio (MP2, CC2, CCSD(T)) calculations to investigate geometrical and electronic structures as well as stabilities of the DOTA ligand (1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid, H_4DOTA) with tetravalent actinide ions An^{4+} (An = Th, Pa, U, Np, Pu) in the gas phase and aqueous solution, and the hydration of Ln(IV)/An(IV) ions M^{4+} (M=Ce, Tb, Th, Pa, U, Np, Pu) as well as uranyl, among others. Excellent agreement is obtained with experimental data/evidence. The reliability of f-in-core pseudopotentials is tested and some problems of an explicit treatment of open f shells by f-in-valence pseudopotentials or at the all-electron level within density functional theory are discussed.

L-P4011
Bosonic Quantum Error Correction: Simpler Structures, Stronger Protection
Ye-Xiong Zeng

Does better quantum error correction necessarily require more complex encodings and control? The rich structure of bosonic quantum states offers new opportunities to address this question. This talk explores how machine learning and physical insight can uncover resource-efficient encodings and recovery mechanisms. Beginning with approximate autonomous quantum error correction, we show how reinforcement learning identifies effective protection schemes with simple interactions. Neural-network-based design extends this approach to approximate Gottesman–Kitaev–Preskill (GKP) codes, achieving improved error correction with fewer squeezed coherent-state components. Superpositions of squeezed Fock states offer a complementary route, combining a compact encoding structure with protection against both photon loss and dephasing, even at moderate squeezing. Together, these results illustrate how carefully designed encodings and recovery dynamics can strengthen quantum information protection while reducing implementation complexity.