ACKNOWLEDGMENTS

The Organizing Committee expresses its gratitude to the Hunan Normal University for hosting this conference and to all the sponsors.

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Brief overview of

Quantum International Frontiers 2018

This meeting is intended to be the first 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 80th anniversary of the founding of Hunan Normal University. For the interested non-Chinese reader: the red and black shapes in the header logo from the website together form the Simplified Chinese character meaning 'start'. The inclusion of the ruby is to signify the 80th anniversary of Hunan Normal University.

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,

Professor Samantha Jenkins (苏曼) Samantha Jenkins.

http://beaconresearch.org
http://www.quantum-int.org/2018/

2013 Chinese Government Friendship Award recipient
2012 6th Xiaoxiang Friendship Award recipient
2010 100 Talent of Hunan Award recipient

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 17-21, 2018

Changsha, China

Scientific programs arranged by day

Arrangement of the Conference

The Timing and Location of the Conference

- 18th, Oct. 08:00 - 08:30 Opening Ceremony: Changsha Room, 4th Floor
- 18th - 21th, Oct. The **Frontiers**/**Pedagogical**/Invited Lectures will be given in Changsha Room, 4th Floor
- 19th, Oct. 19:00 The Poster Session will be held in Changsha Room, 4th Floor

Dining Room of the Conference

- 16th - 21th, Oct. Lunch and Dinner are provided free of charge during the conference, at the Ballroom, 2nd Floor

Contact Information：

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Conference Registration

Wednesday, 17 October, 2018

13:00 to 18:00

Fenglin Hotel, Lobby of the hotel

Opening Ceremony

Thursday, 18 October, 2018 Changsha Room

Chair: Steven Robert Kirk

08:00 to 08:30

Chair’s speech:
Samantha Jenkins (Chair of the Quantum International Frontiers)
Welcome speech:
Le-Man Kuang (Vice-President of Hunan Normal University)

08:30 to 08:45

Take a conference photo (Front Square of the Hotel)

Thursday, 18 October, 2018 A.M Changsha Room

Chair: Yasuteru Shigeta

09:00 to 10:00 **Frontier Lecture**
Akitomo Tachibana (Kyoto University Kyoto, Japan)
Quantum Mechanics: 100 Years of Mystery Solved

10:00 to 10:30 **Tea break**

10:30 to 11:15 **Pedagogical lecture**
Frank E. Harris (The University of Utah, Utah, U.S.A)
Fully quantum non-adiabatic dynamics in the adiabatic representation

11:15 to 11:45
Jie-Ci Wang (Hunan Normal University, Changsha, China)
Quantum coherence and steering in relativistic settings

12:00 **Lunch**

Chair: Frank E. Harris

14:00 to 14:45 **Pedagogical lecture**
Martin Quack (Swiss Federal Institute of Technology Zurich, Switzerland)
Fundamental Symmetries and their Violations in Molecular Quantum Physics

14:45 to 15:15
Lucas Visscher (Vrije Universiteit Amsterdam, Amsterdam, The Netherlands)
Implementation and Applications of Relativistic Coupled Cluster Theory

15:15 to 15:45
Samantha Jenkins (Hunan Normal University, Changsha, China)
Next Generation QTAIM

16:15 to 16:45 **Tea break**

16:45 to 17:15
Wei-Tao Liu (National University of Defense Technology, Changsha, China)
Second-Order Correlation in Time Domain and Its Applications

18:00 **Dinner**

Friday, 19 October, 2018 A.M Changsha Room

Chair: T. Daniel Crawford

09:00 to 10:00 **Frontier Lecture**

Piotr Piecuch (Michigan State University, East Lansing, U.S.A)

Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations

10:00 to 10:30 **Tea break**

10:30 to 11:15 **Pedagogical lecture**

Malgorzata Biczysko (Shanghai University, Shanghai, China)

Nuclear Quantum Effects in Vibrational and Electronic Spectra: the Role of Band Positions and Transition Intensities

11:15 to 11:45

Sergei Manzhos (National University of Singapore, Singapore)

Rectangular collocation for electronic Schrödinger equation

12:00 **Lunch**

Chair: Nawee Kangwan

14:00 to 14:45 **Pedagogical lecture**

Thanyada Rungrotmongkol (Chulalongkorn University, Bangkok, Thailand)

Atomic-level insight into biological processes of molecular recognition, protein dynamics and catalytic origin of enzyme catalysis

14:45 to 15:15

Cho-Hong Lee (Sun Yat-Sen University, Canton, China)

Topological states in periodically modulated systems

15:15 to 16:00 **Pedagogical lecture**

Marco A. C. Nascimento (Federal University of Rio de Janeiro, Rio de Janeiro, Brazil)

The Consequences of Neglecting Permutation Symmetry in the Description of Many-Electron Systems

16:15 to 16:45 **Tea break**

Chair: Xion-Jun Liu

16:45 to 17:15
Jian Liu (Peking University, Beijing, China)
Trajectory-Based Approaches for Quantum Statistics and Quantum Dynamics

17:15 to 18:00 **Pedagogical lecture**
Yasuteru Shigeta (University of Tsukuba, Tsukuba, Japan)
QM/MM analyses on Metalloenzymes and beyond

18:00 **Dinner**

Chair: Steven R. Kirk

19:30 to 22:00
Poster Session see page 9 for details

Saturday, 20 October, 2018 A.M Changsha Room

Chair: Sergei Manzhos

09:00 to 09:30

Mingxing Chen (Hunan Normal University, Changsha, China)

Giant spin-orbit splittings in interface-engineered monolayers

Effects of magnetic dopants and interface oxygen vacancies in FeSe-based superconductors

09:30 to 10:00

Jie-Qiao Liao (Hunan Normal University, Changsha, China)

Generalized Ultrastrong Optomechanics

10:00 to 10:30 **Tea break**

10:30 to 11:15 **Pedagogical lecture**

Paul W. Ayers (McMaster University, Hamilton, Ontario, Canada)

Strong Electron Correlation

Flexible Wavefunction Ansatze for N-electron Systems

11:15 to 12:00

Jian Li (National University of Defense Technology, Changsha, China)

Longitudinally modulated superconducting transmon qubit

12:00 **Lunch**

Chair: Paul W. Ayers

14:00 to 14:30

Xiong-Jun Liu (Peking University, Beijing, China)

Non-equilibrium classification of topological quantum phases

14:30 to 15:00

Haitao Quan (Peking University, Beijing, China)

Path Integral Approach to Work in Quantum Thermodynamics

15:00 to 16:15 **Pedagogical lecture**

T. Daniel Crawford (Virginia Tech, U.S.A)

The Mysteries of Chirality, Solvation, and Optical Activity

16:15 to 16:45 **Tea break**

Chair: Xin-Hua Peng

16:45 to 17:15
Jeffrey R. Reimers (Shanghai University, China)
Design of TADF-Utilizing OLEDs

17:15 to 18:00
Qiong Chen (Hunan Normal University, Changsha, China)
Hyperpolarization with NV centers in diamond

18:00 **Dinner**

Sunday, 21 October, 2018 A.M Changsha Room

Chair: Yu-xi Liu

09:00 to 10:00 **Frontier Lecture**
Xin-Hua Peng (University of Science and Technology of China, Hefei, China)
Experimental quantum simulations towards exotic many-body quantum physics with nuclear spins

10:00 to 10:30 **Tea break**

10:30 to 11:00
Mustafa Eginligil (Nanjing Tech University, Nanjing, China)
Light polarization sensitive 2D materials and hybrid structures

12:00 **Lunch**

Chair: Hai-Tao Quan

14:00 to 14:30
Yu-xi Liu (Tsinghua University, Beijing, China)
Nonlinear quantum optical phenomena in three-level superconducting quantum circuits

14:30 to 15:00
Ping-Xing Chen (National University of Defense Technology, Changsha, China)
Scalable ion-based quantum information processing

15:00 to 16:15 **Pedagogical lecture**
Zhi-Hui Peng (Hunan Normal University, Changsha, China)
Resonance Fluorescence from an Artificial Atom Strongly Coupled to a Cavity

16:15 to 16:45 **Tea break**

Chaired by Martin Quack

16:45 to 17:30 **Pedagogical lecture**
Nawee Kungwan (Chiang Mai University, Thailand, China)
Proton Transfer in the Excited State: Photophysics of Chromophores, fluorescent Probes and Luminescent Materials

Closing Ceremony

Chair: Samantha Jenkins

17:30 to 18:00
Award the Quantum Frontiers Graduate Prizes.
See you at Quantum International Frontiers II

Poster Session

Friday, 19 October, 2018 19:30 Changsha Room

Chair: Steven R. Kirk

P-001

Musen Li (Shanghai University, Shanghai, China)
Easy Ways Towards to the Proper Van der Waals attraction in 2D Systems

P-002

Stefano Fabris (Istituto Officina dei Materiali, Italy)
Modelling the Effects of Chemical Environments on Supported Catalysts

P-003

Xinxing Li (Shanghai University, Shanghai, China)
Simulation of fluorescent dyes optical properties

P-004

Mohamed Amin Ibrahim (Shanghai University, Shanghai, China)
Identification of Amino-Acids Conformers by Vibrational Fingerprints

P-005

Mingzhu Sheng (Shanghai University, Shanghai, China)
Investigation of the hydrogen bonding in serine: a computational spectroscopy study

P-006

Chong Shu (Shanghai University, Shanghai, China)
Accurate determination of energies and molecular structures for isolated small peptides

P-007

Yanting Xu (Shanghai University, Shanghai, China)
Quantum-based refinement of biomacromolecules: the Q|R route

P-008

Hongli Zhang (Shanghai University, Shanghai, China)
The Role of Dispersion and Anharmonic Corrections in Conformational Analysis of Flexible Molecules

P-009

Shanghua Xing (Nagoya University, Nagoya, Japan)
The Influence of Chemical Substituents on Linker Rotational Behaviors in Pillar-layered MOFs by Computational Study

P-010

Likun Yang (Shanghai University, Shanghai, China)
The Lithium Dimer Cation as a Probe for Attosecond Spectroscopy

P-011

Ya-Ju Song (Chinese Academy of Engineering Physics, Beijing, China)
Controlling Decoherence Speed Limit of a Single Impurity Atom in a Bose-Einstein-condensate Bath

P-012

Freda Jean Mwasha (Heriot-Watt University, Scotland, UK)
Excited States of Squaraines via Linear and Non-Linear Electronic Absorption

P-013

Zizhen Rao (Nagoya University, Nagoya, Japan)
Tacticity Prediction of Poly(methyl methacrylate) from Radical Polymerization via Red Moon Methodology

P-014

Alireza Azizi (Hunan Normal University, Changsha, China)
Attractors in Small Charged Lithium Clusters, Li_m^q (m = 2-5, q = ±1), with QTAIM and the Ehrenfest Force Partitioning

P-015

Alireza Azizi (Hunan Normal University, Changsha, China)
A Vector-Based Representation of the Chemical Bond for Predicting Competitive and Non-Competitive Torquoselectivity of Thermal Ring-Opening Reactions

P-016

Roya Momen(Hunan Normal University, Changsha, China)
Role of Weak Interactions in Characterizing Peptide Folding Preferences Using a QTAIM Interpretation of the Ramachandran Plot (ϕ-ψ)

P-017

Roya Momen (Hunan Normal University, Changsha, China)
Exploration of the Forbidden Regions of the Ramachandran Plot (ϕ-ψ) with QTAIM

P-018

Xin Bin (University of Odessa, Odessa, Ukraine)
Next-Generation Quantum Theory of Atoms in Molecules for the Ground and Excited States of the Penta-2,4-dieniminium Cation (PSB3)

P-019

Weijie Huang (Hunan Normal University, Changsha, China)
Next-Generation Quantum Theory of Atoms in Molecules for the Ground and Excited States of Fulvene

P-020

Weijie Huang (Hunan Normal University, Changsha, China)
A Vector-Based Representation of the Chemical Bond for the Normal Modes of Benzene

P-021

Weijie Huang (Hunan Normal University, Changsha, China)
QTAIM and Stress Tensor Bond-path Framework Sets for the Ground and Excited States of Fulvene

P-022

Weijie Huang (Hunan Normal University, Changsha, China)
The 3-D Bonding Morphology of the Infra-Red Active Normal Modes of Benzene

P-023

Jiahui Li (Hunan Normal University, Changsha, China)
A Vector-Based Representation of the Chemical Bond for the Substituted Torsion of Biphenyl

P-024

Jiahui Li (Hunan Normal University, Changsha, China)
Stress Tensor Eigenvector Following with Next-Generation Quantum Theory of Atoms in Molecules

P-025

Jiahui Li (Hunan Normal University, Changsha, China)
Consequences of Theory Level Choice Evaluated with New Tools from QTAIM and the Stress Tensor for a Dipeptide Conformer

P-026

Tian Tian (Hunan Normal University, Changsha, China)
Next-Generation Quantum Theory of Atoms in Molecules for the Ground and Excited State of the Ring-Opening of Cyclohexadiene (CHD)

P-027

Tianlü Xu (Hunan Normal University, Changsha, China)
Consequences for Stereochemistry of Locating the Chirality-Helicity Equivalence in the S and R Stereoisomers of Lactic Acid

P-028

Xiaobao Liu (Hunan Normal University, Changsha, China)
Relativistic motion enhanced quantum estimation of κ-deformation of spacetime

P-029

Zhuang Zhao (Hunan Normal University, Changsha, China)
Strong exciton-photon coupling in solution grown CsPbBr3 micro/nanowires

P-030

Qi Zheng (Hunan Normal University, Changsha, China)
Surface polarons and optical micro-cavity modulated broad range multi-mode emission of Te-doped CdS nanowires

P-031

Heyu Zhu (Hunan Normal University, Changsha, China)
The preferred slip plane of nuclear material of Hafnium: A first-principles study

P-032

Fen Zou (Hunan Normal University, Changsha, China)
Photon blockade effect in a coupled cavity system

P-033

Cao Zhou (Hunan Normal University, Changsha, China)
Amorphous Co-Pi anchored on TiO_2/CdSe nanowire arrays for efficient photoelectrochemical hydrogen production

P-034

Jiansheng Dong (Hunan Normal University, Changsha, China)
The effect of alloying on the band engineering of two-dimensional transition metal dichalcogenides

P-035

Lijuan Hu (Hunan Normal University, Changsha, China)
Concurrence of Two Atoms in a Rectangular Waveguide：Linear Approximation

P-036

Yafeng Jiao (Hunan Normal University, Changsha, China)
Nonlinear optomechanics with gain and loss: amplifying higher-order sideband and group delay Spectroscopy of Atoms and Ions

P-037

Chao Kong (Hunan Normal University, Changsha, China)
Controlling chaotic spin-motion entanglement of ultracold atoms via spin-orbit coupling *Olga Yu.*

P-038

Denggao Lai (Hunan Normal University, Changsha, China)
Simultaneous cooling of coupled mechanical resonators in cavity optomechanics

P-039

Xiaolong Li (Hunan Normal University, Changsha, China)
Soft X-ray activated $NaYF_4$: Gd/Tb scintillating nanorods for in vivo dual-modal X-ray/X-rayinduced optical bioimaging

P-040

Zhen Li (Hunan Normal University, Changsha, China)
Collapse and revival of quantum entanglement in a microscopic-macroscopic system consisting of two Rydberg impurities and a Bose-Einstein condensate

P-041

Shan Liu (Hunan Normal University, Changsha, China)
Symmetrical metallic and magnetic edge states of monolayer 1T-PtX2(X=S、Se)

P-042

Yanjun Liu (Hunan Normal University, Changsha, China)
Fringe visibility and distinguishability in two-path interferometer with an asymmetric beam splitter

P-043

Wangjun Lu (Hunan Institute of Engineering, Xiangtan, China)
Nonlinear Dicke Quantum Phase Transition and Its Quantum Witness in a Cavity-Bose–Einstein-Condensate System

P-044

Yi Ren (Hunan Normal University, Changsha, China)
Negative Poisson's ratio in monolayer blue phosphorene nanoribbon with edge sulfur passivation

P-045

Lijuan Sheng (Hunan Normal University, Changsha, China)
Sensitivity enhanced refractive index sensor by reducing the influence of in-plane wavevector in photonic spin Hall effect

P-046

Ao Zhang (Hunan Normal University, Changsha, China)
Effect of In doping on the topological surface states of Bi2Se3

P-047

Liang Zhang (Hunan Normal University, Changsha, China)
Geometrical effect of thermal conductivity in 2D silicon flms with periodic nanopores

P-048

Zhe Zhang (Hunan Normal University, Changsha, China)
Band Modulation of Black Phosphorus and Molybdenum Disulfide Van Der Waals Heterojunction: Twist and Electric Field Effects

P-049

Zhenluan Xue (Hunan Normal University, Changsha, China)
Non-invasive through-skull brain vascular imaging and small tumor diagnosis based on NIR-II emissive lanthanide nanoprobes beyond 1500 nm

Abstracts for Oral Presentations

Quantum Mechanics: 100 Years of Mystery Solved!

Akitomo Tachibana

Introduction
- Double-slit phenomenon
Theory
  - Time-dependent Hamiltonian of QED
  - Alpha-oscillator theory
  - Thermalization
  - Time-dependent renormalization
  - Dual Cauchy problem
Measurement problem
  - Quantum mechanics (QM) vs Quantum Electrodynamics (QED)
  - Double-slit phenomenon, EPR measurement, and more …
Conclusion

Computationally Convenient Formulation of Open-Shell Molecular Orbital Theory

Frank E. Harris

Computationally convenient formulas are presented for the matrix elements of the identity and of one- and two-electron operators, for open-shell spin-projected wave functions built from orthogonal spatial orbitals. The formulas explicitly show the coefficients of the one- and two-electron integrals involved, and are not much more complicated than the closed-shell formulas in common use. Examples of the use of the formalism are included.

Quantum coherence and steering in relativistic settings

Jieci Wang

Quantum correlations and quantum coherence are two fundamental concepts in quantum theory. While quantum correlations characterize the quantum features of a bipartite or multipartite system, quantum coherence was defined for the integral system. From a practical point of view, quantum correlations and quantum coherence are also invaluable physical resources for quantum information and computation tasks, hence remain research focuses since the early days of quantum mechanics. This talk is an overview of our recent studies for quantum coherence and steering in relativistic settings, including their behaviors of quantum coherence under Unruh-Hawking thermal noise, and satellite-based quantum steering under the influence of space-time curvature of the Earth.

Fundamental Symmetries and their Violations in Molecular Quantum Physics

Martin Quack

Symmetries and asymmetries play a particular role in physics The so called „standard model of particle physics“ (SMPP) reaches in fact far beyond particle physics and can be considered as the current general quantum physical theory of matter and radiation and their interactions. It also provides a “standard model” for atoms, molecules and clusters and molecular quantum physics in general. In the lecture we shall start briefly with a broad picture connecting particle physics with molecular physics in particular in relation to fundamental symmetries and we then introduce basic concepts of molecular structure and dynamics as derived from spectroscopy and kinetics [1].

The general concepts will be illustrated with examples including also quantum mechanical tunneling processes as relevant to our understanding of molecular structure and dynamics of hydrogen bonded complexes as well as chiral and achiral molecules. We briefly discuss most recent progress relating high energy physics to molecular physics through fundamental symmetries and symmetry violations as for example in the very new kinetic process of the time evolution of parity in isolated chiral molecules predicted by theory and perhaps in reach of current experiments. We shall conclude with a brief outlook on “astrobiology” as possibly accessible through spectroscopic observation of chiral molecules. Background reading can be found in [2-9].

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Implementation and Applications of Relativistic Coupled Cluster Theory

Lucas Visscher

While demonstrated to be one of the most accurate electronic structure methods, application of relativistic coupled cluster theory has been limited by the computational scaling of the method. The key algorithm is characterized by large tensor contractions that are demanding in terms of the required memory and in operation count. These same characteristics make the method, however, very well suited for efficient execution on GPU-accelerated massively parallel computer systems. In this presentation I will discuss the restructuring of the relativistic DIRAC program that is necessary to fully utilize the potential of such supercomputers. Besides discussing the technical aspects of the new implementation, I will also present the application of the new code in actinide chemistry. Time permitting, I will furthermore discuss complementary developments in relativistic coupled cluster theory: the application of linear scaling techniques and the calculation of molecular properties.

Next Generation QTAIM

Samantha Jenkins

QTAIM and the stress tensor theory have recently been developed to include a broad range of chemical and physical environments that including:

- New interpretation of the Ramachandran plot applicable to peptides and molecular motors [1].
- The normal modes of vibration of benzene in a stress tensor space [2].
- The dynamics of fast and slow trajectories of a light-driven rotary molecular motor explained by sticky bonding interactions [3].
- Understanding fatigue and photochromism of the S_1 excited state of diarylethenes [4].
- The functioning of doped azophenine switches in a stress tensor space.
- Distinguishing and quantifying the torquoselectivity in competitive ring-opening reactions [5].
- Isomerization of the RPSB chromophore in the gas phase along the torsional pathways using QTAIM [6].
- Investigation of stereochemistry to show anisotropy from QTAIM eigenvectors.
- Function and existence of the non-nuclear attractor (*NNA*) for a series of small charged lithium clusters [7].
- A new vector based interpretation of the chemical bond [8], see **Figure 1**.

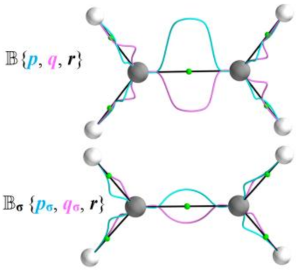

Figure 1. The electronic stress tensor has been identified as useful for the prediction of chemical reactivity due to the ability to determine the most preferred directions to move the bonds corresponding to qualitative changes in the molecular electronic structure. The need to use a directional approach along the entire bond as well as the insufficiency of the sole use of scalar measures for capturing the nature of the stress tensor within the QTAIM partitioning is demonstrated.

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Second-Order Correlation in Time Domain and Its Applications

Wei-Tao Liu

Second-order correlation has been widely used in the field of ghost imaging, which allows achieving image of the objects with a single-pixel detector, providing the robustness against harsh environment. In typical ghost imaging, spatial correlation is used. We extended the idea of ghost imaging into time domain, to perform computational ghost imaging in time domain such that we can reconstruct a fast signal with a much slower detector. Furthermore, by introducing second-order time correlation into typical ghost imaging, the image quality can be greatly enhanced under strong background noise. In particular, based on second-order correlation between two photons, with Hong-Ou-Mandel interference, temporal amplitude and phase of one photon can be precisely measured, which also shows robustness against noise.

Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations

Piotr Piecuch

One of the main goals of electronic structure theory is precise *ab initio* description of increasingly complex polyatomic systems. It is widely accepted that size extensive methods based on the coupled-cluster (CC) theory are excellent candidates for addressing this goal. Indeed, when applied to molecular properties and chemical reaction pathways, the CC hierarchy, including CCSD, CCSDT, CCSDTQ, etc., rapidly converges to the limit of the exact, full configuration interaction (FCI), diagonalization of the Hamiltonian, allowing one to capture the relevant many-electron correlation effects in a conceptually straightforward manner through particle-hole excitations from a single Slater determinant. One of the key challenges has been how to incorporate higher–than–two-body components of the cluster operator, needed to achieve a quantitative description, without running into prohibitive computational costs of CCSDT, CCSDTQ, and similar schemes, while eliminating failures of the more practical perturbative approximations of the CCSD(T) type in multi-reference situations, such as chemical bond breaking. In this talk, we examine a radically new way of obtaining accurate energetics equivalent to high-level CC calculations, even when electronic quasi-degeneracies and higher–than–two-body clusters become significant, at the small fraction of the computational cost, while preserving the black-box character of single-reference computations. The key idea is a merger of the deterministic formalism, abbreviated as CC(P;Q) [1,2], with the stochastic CI [3,4] and CC [5] Quantum Monte Carlo (QMC) approaches [6]. We also demonstrate that one can take the merger of the stochastic and deterministic ideas to the ultimate level and use it to accelerate convergence of FCIQMC calculations, enabling accurate extrapolations of the exact, FCI, energetics based on the early stages of FCIQMC propagations [7]. The advantages of the new methodologies will be illustrated by molecular examples, where the goal is to recover the nearly exact, CCSDT and CCSDTQ, and exact, FCI, energetics, including bond breaking in F_2 and H_2O and the automerization of cyclobutadiene.

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Nuclear Quantum Effects in Vibrational and Electronic Spectra: the Role of Band Positions and Transition Intensities

Malgorzata Biczysko

Spectroscopic techniques are nowadays the most advanced tools playing a prominent role in the experimental investigation of static and dynamic properties of all kinds of systems, especially when different spectroscopic measurements are combined together to offer a comprehensive picture. Understanding of processes and phenomena can be complemented by computational studies allowing for a direct vis-à-vis comparison between experimental and simulated spectra. Concerning 'fingerprint' vibrational features in infrared (IR), Raman, Resonance Raman, UV-vis or fluorescence spectra, including also their chiral counterparts, it is crucial to go beyond the most standard computational procedures by including nuclear quantum anharmonic and/or vibro-electronic effects on both band positions and transition intensities.

I will discuss efficient procedures, allowing simulation of realistic spectra band-shapes for medium-to-large systems, which are based on the generalized second-order Vibrational Perturbation and time-independent Franck-Condon and Herzberg-Teller computations in conjunction with density functional theory (DFT)/coupled cluster (CC) schemes and their extension to the excited electronic states.

Rectangular collocation for electronic Schrödinger equation

Sergei Manzhos

Rectangular collocation was recently proposed as a way to solve the vibrational Schrödinger equation with a relatively small number of potential samples and basis functions. One of the advantages of the method is possibility to use any basis functions as there is no requirement of integrability or of smoothness except in the vicinity of collocation points. Another advantage is possibility of using any desired distribution of collocation points.

Here, we show that thanks to these advantages rectangular collocation can be effective for solving the electronic Schrödinger equation (ESE). We compute several solutions of the ESE for the H atom and the H_2^+ cation and several solutions of a Kohn-Sham equation for CO and H_2O. In all cases, we achieve millihartree accuracy. We use basis functions that are similar to Slater type orbitals which are most effective for full-potential problems. They are rarely used with the variational method, where often Gaussian-like or plane wave basis functions are used due to the simplicity of integration, but Slater-type functions present no integration issues when used with collocation. We also show that it is advantageous to select collocation points with a distribution emphasizing low-energy regions of the (effective) potential, which is easy to achieve with collocation.

Atomic-level insight into biological processes of molecular recognition, protein dynamics and catalytic origin of enzyme catalysis

Thanyada Rungrotmongkol

Based on fundamental mathematics and physics applied on protein structure, computational biology offers the potential of uniquely detailed, atomic-level insight into biomolecular structure and function, mechanisms of drug action, source of microbial resistance and mechanistic insights into enzyme catalysis. Successful examples in several biological problems are given as follows. In the outbreak of influenza A(H1N1)pdm 2009, models of the neuraminidase and M2-channel were built from the available 3D structures and the genomic sequence data of virions isolated from infected patients in southern California, A/California/04/2009 (H1N1). From molecular dynamics (MD) results, the stockpiling oseltamivir can inhibit this virus mainly through electrostatic interaction with neuraminidase, while the adamentanes cannot block the proton transfer through M2-channel due to S31N mutation. Using computer-aided drug design techniques, the newly designed and screened compounds specifically targeted at neuraminidase, dengue E protein, DNA topoisomerase and EGFR have shown high activity in enzyme and/or cell based assays. Protein conformational change upon ligand binding and molecular recognition in between drug/inhibitor-protein, peptide-protease, peptide-MHC class I/II, and host membrane sialylated glycans-glycoprotein have been revealed by MD and principle component analysis. Mechanistic details of enzyme-catalyzed reactions on proteolytic cleavage in viral and host proteases, DNA polymerization in HIV-1 RT, and Michael addition in thymidylate synthase was investigated by combined QM/MM techniques, which could describe the enzymatic reaction, catalytic rate constant, crucial residues, and short-lived species (transition states and intermediates) in a more accurate way. Fundamental understanding of molecular behaviors of protein in different conditions, i.e., protein motion and flexibility, dynamics biochemical interactions, enzyme mechanisms and effects of mutations at atomistic level are helpful to guide and speed up the early-stage drug discovery process.

Topological states in periodically modulated systems

Chaohong Lee

Topology is the mathematics of conserved properties under continuous deformations. The combination of topology and physics provides unique insight into quantum Hall states, materials, and devices. On the other hand, periodic modulations are extensively used to modulate various physical systems. In this talk, I will present our recent works on topological states in periodically modulated system: (1) the Thouless pumping of light in modulated wave guides [Laser Photon. Rev. 10, 995 (2016)], (2) the Thouless pumping of interacting Bose atoms in modulated optical lattices [Phys. Rev. A 95, 063630 (2017)], and (3) the topological Floquet edge states in modulated photonic lattices [Phys. Rev. A 98, 013855 (2018)].

The Consequences of Neglecting Permutation Symmetry in the Description of Many-Electron Systems

Marco A. C. Nascimento

The consequences of neglecting the permutation symmetry of the Hamiltonian of many-electrons system is examined. From the comparison of wave functions based on methods which take (Generalized Valence Bond-GVB) and do not take (Hartree-Fock) the permutation symmetry into account it is shown that neglecting the permutation symmetry leads to false concepts, misinterpretations and unjustifiable approximations when dealing with many-electrons systems, atoms and molecules. In particular, it is shown how the double occupancy of atomic and molecular orbitals, the exchange integral, the correlation energy and the so-called “non-dynamic” correlation energy are related to neglecting the permutation symmetry.

Trajectory-Based Approaches for Quantum Statistics and Quantum Dynamics

Jian Liu

Unraveling nuclear quantum effects (zero point energy, tunneling, decoherence, coherence, etc.) in dynamic, spectroscopic and thermodynamic properties of complex systems has presented challenging frontiers in modern physical chemistry. We will present an introduction to the theories and to our recent progress. The pedagogical talk consists of two parts: One is on an efficient unified theoretical scheme for performing path integral molecular dynamics for obtaining thermodynamic properties, the other is on three unified frameworks in the phase space formulation of quantum mechanics for developing trajectory-based methods for studying dynamic and spectroscopic properties.

QM/MM analyses on Metalloenzymes and beyond

Yasuteru Shigeta

Proteins are macromolecular compounds with extremely complex structures and drive various biological functions *in vivo* such as molecular recognition, signal transduction, enzymatic reaction, and etc. Since it is expected that there is a correlation between the structure and the function (structure-function relationship), the three-dimensional structures of many proteins have been clarified by experimental methods such as X-ray diffraction experiment and nuclear magnetic resonance method (NMR). Especially, dynamic information of a protein is recently obtained by state-of-the-art experimental techniques such as X-ray free electron laser, cryo-electron microscopy, AFM and STM, and etc., which enable ones to elucidate protein functions in detail. Under such circumstances, theoretical calculations become more important to confirm experimental facts at the microscopic level and predict its vital role. With recent progress in both supercomputer architectures and computational methodologies to analyze biomolecules, the field of chemical reaction analysis occurring in vivo has made remarkable progress. In this seminar, molecular dynamics simulations and first-principles methods for analyzing biological phenomena are reviewed. Especially, QM/MM analyses on metalloenzymes and problems are discussed. As a future prospect, trials of methodologies beyond QM/MM are introduced.

Effects of magnetic dopants and interface oxygen vacancies in FeSe-based superconductors

Mingxing Chen

The newly discovered high-Tc Fe-based superconductors, i.e., FeSe monolayer on SrTiO3 and (Li1-xFexOH)FeSe have attracted great interest in the investigations of their electronic structures and explorations of the underlying mechanism for the high-Tc superconductivity. In this talk I will describe a band unfolding technique called k-projection method for doped materials and interfaces. Then we apply this method to investigate the effects of oxygen vacancies on the electronic bands at the interface of between FeSe thin films and SrTiO3 and the effects of Fe dopants on the electronic bands of (Li0.8Fe0.2OH)FeSe. We find that the interfacial oxygen vacancies as well as the Fe impurities doped into the LiOH layers cause electron donation to the FeSe layers, significantly changing the profile of bands around the Fermi level. We compare the k-projected bands with ARPES results and discuss effects of surface, spin-orbit coupling and different magnetic orderings on the comparison.

Generalized Ultrastrong Optomechanics

Jie-Qiao Liao

We propose a reliable scheme to realize a generalized ultrastrong optomechanical coupling in a two-mode cross-Kerr-type coupled system, where one of the bosonic modes is strongly driven. The effective optomechanical interaction takes the form of a product of the photon number operator of one mode and the quadrature operator of the other mode. The coupling strength and quadrature phase are both tunable via the driving field. The coupling strength can be strongly enhanced to reach the ultrastrong-coupling regime, where the few-photon optomechanical effects such as photon blockade and macroscopically distinct quantum superposition become accessible. The presence of tunable quadrature phase also enables the implementation of geometric quantum operations. Numerical simulations show that this method works well in a wide parameter space. We also present an analysis of the experimental implementation of this scheme.

Strong Electron Correlation

Paul W. Ayers

Since the electronic Schrödinger equation is too complicated to be soluble for most interesting molecules, it is important to develop practical approximations that provide accurate models for the behavior of electrons within molecules. The difficulty of the underlying problem implies that these models are necessarily limited to certain special cases. For example, it is relatively easy to describe cases where the electrons in a molecule move nearly independently, so that the motion of one electron does not affect others very much. When this is not true, many of our conceptual precepts lose their utility because the notion of an electron configuration, and even the concept of orbitals, ceases to be relevant. In addition, when the independent-electron approximation breaks down, most conventional computational methods become unreliable. In this seminar, I will discuss quantum models for strongly correlated molecules, focusing on alternatives to orbital-based models. Specifically, I will discuss models based on tensor-product decompositions, complexity-based truncations, and composite particles.

Longitudinally modulated superconducting transmon qubit

Jian Li

In this talk, we present the experimental and theoretical results of a superconducting qubit, namely a transmon, with time-dependent flux drives. The time-dependent flux drives lead to (longitudinal) modulations of the transmon energy splitting. For pseudo-random telegraph noise modulations, the energy splitting of the transmon jumps stochastically between two discrete values. When the jumps are faster than a dynamical threshold set by the energy splitting displacement, the initially separated spectral lines merge into a single one. This process mimics a striking phenomenon observed originally in NMR spectroscopy, known as the motional averaging. With sinusoidal modulations, we observe complex patterns of additional sidebands in transmon spectra, which can be explained by (microwave) photon-assisted Landau-Zener-Stückelberg interference. We also find that with longitudinal modulation, a transmon + microwave cavity strong coupling circuit QED (which is described by the well-known Jaynes-Cummings model) can be used to simulate ultra-strong coupling even deep strong coupling dynamics.

Non-equilibrium classification of topological quantum phases

Xiong-Jun Liu

Topological phase of matter is now a mainstream of research in condensed matter physics, of which the classification, synthesis, and detection of topological states have brought many excitements over the recent decade while remain incomplete with ongoing challenges in both theory and experiment. In this talk I present a universal dynamical characterization of the topological quantum phases classified by integers, and show its application to detecting topological physics with high precision [1]. The framework of the theory consists of several findings. First, we uncover that classifying a generic d-dimensional (dD) gapped topological phase can reduce to a (d-1)D invariant defined on so-called band inversion surfaces (BISs), rendering a basic bulk-surface duality. Further, we show in quenching across phase boundary the (pseudo)spin dynamics to exhibit unique topological patterns on BISs, which are attributed to the post-quench bulk topology and manifest a dynamical bulk-surface correspondence. The topological phase is then classified by a dynamical topological invariant measured from dynamical spin-texture field on the BISs. Applications to quenching experiments on feasible models are proposed and studied. The dynamical detection with high precision of the topological quantum physics has already been achieved in experiments [2, 3]. The generalization [4] and further interesting issues will be discussed.

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Path Integral Approach to Work in Quantum Thermodynamics

Haitao Quan

Work belongs to the most basic notions in thermodynamics but it is not well understood in quantum systems, especially in open quantum systems. By introducing a novel concept of the work functional along an individual Feynman path, we invent a new approach to study thermodynamics in the quantum regime. Using the work functional, we derive a path integral expression for the work statistics. By performing the $\hbar$ expansion, we analytically prove the quantum-classical correspondence of the work statistics. In addition, we obtain the quantum correction to the classical fluctuating work. We can also apply this approach to an open quantum system in the strong coupling regime described by the quantum Brownian motion model. This approach provides an effective way to calculate the work in open quantum systems by utilizing various path integral techniques. As an example, we calculate the work statistics for a dragged harmonic oscillator in both isolated and open quantum systems.

The Mysteries of Chirality, Solvation, and Optical Activity

T. Daniel Crawford

The optical properties of chiral molecules are among the most challenging to predict, even for state-of-the-art quantum chemical methods because of their delicate dependence on a variety of intrinsic and extrinsic factors, including electron correlation, basis set, vibrational/temperature effects, etc. This task is made even more difficult by solvation, which can have a dramatic impact on even the sign of optical rotation angles or circular dichroism rotational strengths. In this lecture, we will discuss the most recent efforts from our group to attack this problem, including both implicit and explicit solvent models, and the role of reduced-scaling techniques to improve the efficiency of such computations..

Ab initio corrections for density-functional theory energies of excited states of defects in 2D materials

R. Reimers

Defect states in 2D materials present many possible uses but both experimental and computational characterization of their spectroscopic properties is difficult. We provide and compare results from 13 DFT and ab initio computational methods for up to 25 excited states of a paradigm system, the VNCB defect in hexagonal boron nitride (h-BN). Studied include include:
(i) potentially catastrophic effects for computational methods arising from the multi-reference nature of the closed-shell and open-shell states of the defect, which intrinsically involves broken chemical bonds, (ii) dif-fering results from DFT and time-dependent DFT (TDDFT) calculations, (iii) comparison of cluster models to periodic-slab models of the defect, (iv) the starkly differing effects of nuclear relaxation on the various electronic states as broken bonds try to heal that control the widths of photoabsorption and photoemission spectra, (v) the effect of zero-point energy and entropy on free-energy differences, (vi) defect-localized and conduction/valence band transition natures, and (vii) strategies needed to ensure that the lowest-energy state of a defect can be computationally identified. Averaged state-energy differences of 0.3 eV are found between CCSD(T) and MRCI energies, with thermal effects on free energies sometimes also being of this order. However, DFT-based methods can perform very poorly. Simple generalized-gradient functionals like PBE fail at the most basic level and should never be applied to defect states. Hybrid functionals like HSE06 work very well for excitations within the triplet manifold of the defect, with an accuracy equivalent to or perhaps exceeding the accuracy of the ab initio methods used. However, HSE06 underestimates triplet state energies by on average 0.7 eV compared to closed-shell singlet states, while open-shell singlet states are predicted to be too low in energy by 1.0 eV. This leads to miss-assignment of the ground state of the VNCB defect. Long-range corrected functionals like CAM-B3LYP are shown to work much better and to represent the current entry level for DFT calculations on defects. As significant differences between cluster and periodic-slab models are also found, the widespread implementation of such functionals in periodic codes is in urgent need.

Hyperpolarization with NV centers in diamond

Qiong Chen

Magnetic resonance imaging (MRI) has gained widespread use in life-science and medical research, such as cancer diagnosis, recognizing molecular processes and drug discovery. The main limitation is the low signal-to-noise ratio (SNR) resulting from small nuclear polarization. Hyperpolarization (enhancing this polarization by orders of magnitude) is the major tool to overcome this limitation. Traditional hyperpolarization methods are slow and expensive as they require cryogenic temperatures. The Nitrogen-vacancy (NV) centers in diamond own unique optical properties and near perfect optical polarization, which could be used for hyperpolarization as a promising way to improve the SNR by several orders at room temperature without the aforementioned disadvantages. We developed several schemes to hyperpolarize ^{13}C nuclear spins by using NV centers, either inside the diamond or in external molecules, thus bringing innovation from this field to offer radical improvements over the existing technologies for hyperpolarization, enabling cost-effective molecular imaging with nanomolar sensitivity with conventional MRI systems.

Experimental quantum simulations towards exotic many-body quantum physics with nuclear spins

Xin-Hua Peng

Along the lines suggested by Feynman, complex quantum systems can be efficiently simulated on quantum simulators, i.e., programmable quantum systems whose dynamics can be efficiently controlled. Quantum simulations thus offer the possibility to investigate many-body quantum systems that are challenging for simulations on classical computers. Nuclear magnetic resonance is a good test platform for the physical implementation of quantum simulator due to its sophisticated control and precise measurement in multi-qubit experiments. This lecture is an overview of our recent progress on experimental quantum simulation to investigate exotic many-body physics using nuclear spins, including the adiabatic transition in the Wen-plaquette model between two different Z2 topological orders, the measurement of the modular S, T matrices in Kitaev toric code model to identify the Z2 topological order, and information scrambling measured by out-of-time-order correlator. Moreover, we also report a feedback loop scheme between a classical computer and a quantum simulator to tackle the quantum optimal control problem. Our techniques should be useful in establishing quantum simulations for complex many-body physics quantum problems.

Light polarization sensitive 2D materials and hybrid structures

Mustafa Eginligil

We investigated the photocurrent behavior of genuinely 2D material graphene and excitonic physics of valleytronic 2D semiconductors with high valley polarization, by polarized light. In multilayer graphene with restored inversion symmetry and band gap opening, we observed large tunable circular photogalvanic current. In monolayer MoS2 with broken inversion symmetry and strong spin-orbit coupling, we demonstrated large photocurrent dichroism due to the circular photogalvanic effect upon resonant excitation. Additionally, at low temperatures, we observed a crossover from positive magneto-photoconductivity (MPC) to negative MPC of monolayer MoS2 FET devices. This crossover was not observed for bilayer MoS2 FET devices. We explain this observation in terms of illumination and localization effects based on a recent theory. We also characterized optical properties of hybrid structures based on light sensitive biomaterials and atomically thin 2D materials for sensing applications.

Nonlinear quantum optical phenomena in three-level superconducting quantum circuits

Yu-xi Liu

We know that the three-wave mixing cannot be produced in three-level atomic system because of the electric-dipole transition selection rules. In this talk, I will show how a single three-level superconducting artificial atom, e.g., flux qubit circuit, can be used to produce three-wave mixing, frequency conversion, and microwave amplifications of classical microwave fields. And then I will report a proposal for efficient single-photon frequency conversion in the microwave domain using superconducting quantum circuits. In particular, we quantitatively discuss the effects of amplification and the frequency conversion for different types of driving fields. The values and conditions are obtained for the optimal gains of amplification and the optimal conversion efficiencies of microwave conversion.

Scalable ion-based quantum information processing

Ping-Xing Chen

Trapped ion is a promise system for quantum information processing. In this talk, I will introduce briefly our scheme for ions cooling and the method to measure quantum states. Then, I will introduce our chip ion-trap in detail. A chip trap is a promising system for scalable quantum information processing with trapped ions. The stable trapping and transformation of the ions in chip traps are necessary for the preparation and operation of the ions states with high fidelity. We designed a surface-electrode chip trap, and show it has excellent ability of trapping ions. Using some practical experimental operation methods, we have successfully reduced the trap heating rate. As a result, we are able to trap a string of up to more than 50 ions, and get a zigzag structure with 24 ions, and transport trapped ions to different zones. Also we proposed a feedback control method for producing an equidistant ion string in a surface-electrode ion trap. Our system may have applications in large-scale quantum computing, quantum simulation, and phase transition studies.

Resonance Fluorescence from an Artificial Atom Strongly Coupled to a Cavity

Zhi-Hui Peng

We experimentally study the resonance fluorescence from an atom strongly coupled to a cavity in two regimes and the observed Mollow triplets are drastically different from the atom coupled to an open space. In regime 1, a single superconducting artificial atom is strongly coupled to a cavity. In regime 2, one of sidebands of the driven artificial atom is strongly coupled to a cavity. The unusual resonance fluorescence is directly revealed by measuring the emission spectrum from the strongly driven artificial atom which is simultaneously strongly coupled a cavity and an open space. We clearly observed the main features of resonance fluorescence determined not by relaxation rate of the atom but by the coupling strength between the atom and the cavity.

Proton Transfer in the Excited State: Photophysics of Chromophores, fluorescent Probes and Luminescent Materials

Nawee Kungwan

Tautomerization taking place in organic molecules as a bifunctional group through the excited-state proton transfer (ESPT) between proton donor and proton acceptor (either ESIntraPT or ESInterPT with assistance of protic solvent) is one of the most studied and applicatively promising photoreactions. The most remarkable photophysical property of the ESPT molecules is the large Stokes shift of, compared to the normal chromophores. Their applications are found in many fields from fluorescent molecular probes (chemosensors and bioimaging) to luminescent materials (optoelectronic devices). Up to now, extensive spectroscopic and theoretical research studies on the photophysical process of ESPT molecules have been carried out, however their molecular structure-property relationship has not been well understood, particularly the role played by solvent assistance and absorption and fluorescent spectra controlled by chemical modification of well-known ESPT molecules. In this present contribution, we would like to investigate these mentioned properties with the help of quantum-mechanical tools both static calculations and dynamic simulations of some interesting systems.

Poster Abstracts

P-001
Easy Ways Towards to the Proper Van der Waals attraction in 2D Systems
Musen Li

Studies and applications of two-dimensional (2D) systems such as hexagonal boron nitride, graphene and other promising systems have grown exponentially over the past decade. To boost the speed of 2D system studies, many empirical correction methods, such as D3 and many body dispersion (MBD), have been engaged to describe the van der Waals interaction in 2D systems. We compared several van der Waals correction methods (D3, MBD, and layer response theory (LRT)) performance, which will help people to understand the results given by different methods and select the proper van der Waals correction method for the specific 2D system.

P-002
Modelling the Effects of Chemical Environments on Supported Catalysts
Stefano Fabris

Density functional theory calculations are combined with molecular dynamics, ab-initio thermodynamics, metadynamics, and other enhanced-sampling methods to investigate the surface chemistry of sdupported catalysts in a wide range of compositions and environments, ranging from model surfaces at T=0K in vacuum conditions to realistic wet electrodes at finite temperatures. The computational predictions are confirmed by the dedicated synthesis and characterisation of model catalytic systems that mimic nanostractured large-area materials. This allows us to propose guidelines for the design of new materials with increased catalytic efficiency and reduced precious-metal content.

P-003
Simulation of fluorescent dyes optical properties
Xinxing Li

The interpretation and prediction of optical properties of fluorescent dyes can be greatly facilitated by a computational support. For instance, it can help identifying the most interesting chromophores among a large number of potential candidates for the design of new materials or sensors, as well as unraveling the many effects contributing to the overall spectroscopic phenomena.

Viologen derivatives (1,1′-disubstituted-4,4′-bipyridinium cation salts) are characterized by significant color change during the charge transfer reaction, and have been widely studied and applied in the fields of electrochromic display, molecular electronics, solar energy conversion and storage devices, supramolecular host−guest complexes and molecular machines, and colorimetric sensing material. In this work novel viologen derivatives, differing in the geometry structure and aromatic substituents have been obtained experimentally and characterized by spectroscopic and theoretical methodologies. The absorption and emission spectra have been simulated at first by the computation of vertical or adiabatic excitation energies and related transition moments at the TD-CAMB3LYP level, and further convoluted by phenomenological Gaussian distribution functions to mimic the broadening observed in the experimental line-shapes. These results allowed to assign observed experimentally fluorescence red-shift to the keto-enol transition and give indication on enhanced fluorescence of studied viologens. However, thanks to the availability of efficient procedures, simulation of vibrationally-resolved absorption and emission spectra, including environment and temperature effects, have been also performed.

P-004
Identification of Amino-Acids Conformers by Vibrational Fingerprints
Mohamed Amin Ibrahim

Peptide building blocks allow creation of tremendous versatile molecular architectures showing very specific functionalities, with millions of protein variants in human proteome obtained just by the twenty canonical amino acids alone. Among the various types of investigations spectroscopies are the most powerful tools for comprehensive analysis of the properties of amino acids and their oligomers, which show ‘finger-print’ vibrational features in infrared (IR), Raman, Resonance Raman, UV-vis or fluorescence spectra, including also their chiral counterparts However, the conformational flexibility causes also that the results of experimental spectroscopic studies are difficult to interpret. In fact even for the smallest isolated amino-acids, several conformers with specific spectroscopic features, might be concomitantly present in the experimental mixture complicating to link the rich experimental data to the desired information on the molecular structure and properties.

Accurate equilibrium structures, thermodynamic properties and vibrational patterns are essential starting points for the analysis of the spectroscopic properties for molecular systems. In this framework, vibrational corrections to molecular structures and properties or thermodynamic functions can be obtained from the same anharmonic force fields as employed in the determination of vibrational properties. It has been demonstrate that sufficiently accurate anharmonic contributions can be obtained with the second-order vibrational perturbation theory (VPT2) in conjunction with density functional theory (DFT) computations, applying dispersion-corrected hybrid density functionals (especially B3LYP-D3), and including improved descriptions from double hybrid (e.g. B2PLYP-D3) approaches. This approach is applied here to support analysis of novel experimental matrix-isolation IR spectroscopy results for proline, with less stable conformers generated by NIR laser irradiation.

P-005
Investigation of the hydrogen bonding in serine: a computational spectroscopy study
Mingzhu Sheng

A comprehensive analysis of the properties of amino acids oligomers and the detailed characterization of their supra-molecular structure, orientation and dynamics is the basic requirement for understanding the structure-function relationships, which further allow designing specific macromolecular architectures with desired micro- and macroscopic properties. However, it is currently not possible to predict supramolecular behaviour from sequence alone because molecular organization usually depends on the synergistic combination of specific and nonspecific interactions, e.g., ionic, covalent, van der Waals, hydrogen bonding, etc. Among the various types of investigations, spectroscopic techniques are the most powerful tools, thus allowing the direct detection of different binding schemes via microwave (MW) measurements or indirect analysis through ‘finger-print’ vibrational features in infrared (IR), Raman, Resonance Raman, UV-vis or fluorescence spectra, also including their chiral counterparts. In this respect, the most stable conformers of serine represents an interesting case with a structure governed by three or two different type hydrogen bond interactions, namely, O-H…N, O-H…O=C and N-H…O-H, for which both microwave and IR spectra have been measured experimentally. These conformers of serine represent an interesting test case for the determination of improved spectroscopic parameters by means of composite schemes. The present computational study aims at a more accurate determination of the hydrogen-bond characteristics from which the various conformations depend on. Moreover, highly accurate theoretical results of CCSD(T)/CBS quality and available spectroscopic data stand as a reference for benchmarking of DFT approaches, focusing on dispersion-corrected and double-hybrid DFT models.

P-006
Accurate determination of energies and molecular structures for isolated small peptides
Chong Shu

Among biomolecules building blocks amino acids and polypeptides represents the highly flexible molecular systems with several possible structural arrangements. This flexibility is related to the presence of single bonds allowing for conformational freedom. Even for the isolated amino acids, many conformers are possible and several of them can be observed in experiment. Properties of amino acids oligomers depend on their supra-molecular structure, which can be additionally complicated by combination of weak inter- and intra-molecular interactions, as for example hydrogen bonding and dispersion. From just twenty canonical amino acids it is possible to build very different molecular architectures showing specific functionalities, as demonstrated by the number of already known protein structures.

Understanding and prediction of three-dimensional (3D) conformation, important for detection of simplest amino-acids in the interstellar space, prebiotic molecules evolution toward more complex species, polypeptides self-assembly or structure-function relations in proteins, requires reliable theoretical support. Highly accurate methodologies are applicable to small amino acids and polypeptides. These results can be used to check accuracy of less expensive ones, which can be applied to larger and more complex molecular systems. For the latter, the challenging aspects are related not only due to the increasing system size but also the description of all types of weak molecular interactions, and exploration of conformational space which are needed for the correct description of the related three-dimensional structures.

Step-by-step strategy can start from comparison of dispersion-corrected DFT approaches with highly accurate theoretical results of CCSD(T)/CBS quality and state-of-the-art experimental laser ablation molecular beam Fourier transform microwave (LA-MB-FTMW) spectroscopy results for amino acids and small polype

P-007

Quantum-based refinement of biomacromolecules: the Q|R route

Yanting Xu

Protein modeling is largely reliant upon X-ray protein crystallography, electron cryo-microscopy or NMR experiments for obtaining accurate atomic models, which are further deposited in the Protein Data Bank (PDB). Refinement of an atomic model is the final critical step in obtaining accurate three-dimensional structures of bio-macromolecules based on experimental crystallographic or microscopy data. Since the quality of the experimental data (e.g., resolution) is rarely sufficient to utilize these data alone, this step has traditionally relied on parameterized libraries that depict stereochemistry of the molecules in question. Unfortunately, these tools are not well suited for unusual local arrangements of protein in Ramachandran space, description of hydrogen bond interactions or non-typical protein-ligand interactions. In particular, structures obtained using low-to-medium resolution data with the aid of protein structure refinement tools are biased by simple harmonic geometry restraints. By contrast, quantum chemical computations can predict accurate geometries for any well-defined backbone Ramachandran orientation or novel protein-bio-active molecule systems, adding valuable support for detailed analysis of local structural arrangements in proteins, and providing improved or missing data for less understood high-energy or unusual regions. There are several possible applications of quantum-chemistry based approaches, either directly or as reference data for less-expensive methodologies. Here we highlight already feasible yet less-regarded applications to the protein crystallographic refinement, in particular the direct combination of computational and experimental data in quantum refinement procedures.

The methods we are developing in the Q|R project, which is our next generation open-source software package (http://github.com/qrefine), combine experimental data with chemical restraints computed using quantum-chemical methods. These procedures have proven to better describe non-covalent interactions, and are expected to yield more accurate information on the protein structures, e.g. better description of ligand binding.

P-008

The Role of Dispersion and Anharmonic Corrections in Conformational Analysis of Flexible Molecules

Hongli Zhang

Conformational analysis represents a first step toward a detailed characterization and understanding of the structure-function relationships of molecular systems . In this respect spectroscopic experiments on isolated bio- and organic-molecules allow detection of different binding schemes and three-dimensional (3D) conformations without perturbing effects of environment. Detection of multiple 3D-geometries concomitantly present in an experimental mixture can be facilitated by “in situ” structural changes induced either by thermal variations, or the interaction with near-IR (NIR) to ultraviolet (UV) light. These sophisticated experiments need to be supported by accurate and reliable computational studies allowing to link the rich experimental data to the desired information on the structure and properties of complex molecular systems.

Safrole represents a challenging example of a flexible molecule highlighting importance of dispersion interactions and anharmonic effects in the structural, spectroscopic and energetic analysis. Structures of the safrole conformers, their energetics and infrared spectra have been calculated using various computational methods ranging from density functional theory (DFT) to coupled cluster (CC). The best theoretical results were obtained by integrating CCSD(T) energies including complete basis set extrapolation and core-valence corrections with B2PLYP-D3 equilibrium structures and hybrid B2PLYP-D3/B3LYP-D3 anharmonic computations for IR spectra and thermodynamics.

P-009

The Influence of Chemical Substituents on Linker Rotational Behaviors in Pillar-layered MOFs by Computational Study

Shanghua Xing

Utilizing the feature of functionalized MOFs has been revealed as a promising route for precision polymer synthesis. Among MOFs that can tailor polymerization, studies mostly concentrate on the family of flexible pillar-layered framework with the type of [Zn2(BDC)2DABCO]n (BDC = 1,4-benzenedicarboxylates and DABCO = 1,4-diazabicyclo[2,2,2]octane). By utilizing the one-dimensional nanochannel of the MOFs for radical polymerization of poly(methyl methacrylate) (PMMA), the BDC linker (benzene group) functionalization can realize the controllable tacticity of product PMMA polymerization by different substituents (-F, Cl, Br, CH3, NH2, OCH3)1. However, the molecular-level mechanism for the effect of dynamic linker on the polymerization by different substituents is still elusive. X-ray crystallographic structures show small substituent-dependent difference in [Zn2(x-BDC)2DABCO]n (x-BDC is a substituted BDC) structure, except for the rotational behaviors of x-BDC linker by different substituents. As a consequence, we systematically explored the substituent-dependent rotational behaviors by density functional theory (DFT) calculations, where the planarity and rotational barrier were considerably changed. Additionally, the rotation of DABCO had further influence on the trend of the most stable structure by different substituents. This finding can be explained by the difference of local interaction including van der Waals (VDW) repulsion and electrostatic interaction. Our study would contribute to correctly simulate the process of radical polymerization within MOF channel by different substituents.

P-010

The Lithium Dimer Cation as a Probe for Attosecond Spectroscopy

Likun Yang

Attosecond spectroscopy presents possibilities for the control of chemical reaction dynamics and products, and herein we consider one of the three simplest paradigm systems: core-ionized Li2+. Its properties are depicted using equations of motion coupled-cluster (EOM-CCSD) calculations as well as complete-active-space self-consistent-field (CASSCF) calculations, focusing on the primary expected electronic resonance of interest between the and components of the ground-state core-ionized dimer, as well as close-lying resonances with states displaying additional 2s 2p excitation. All higher-energy states involving mixed 1s-2s ionization are also detailed, as well as the electron-electron entanglement that they manifest.

P-011

Controlling Decoherence Speed Limit of a Single Impurity Atom in a Bose-Einstein-condensate Bath

Ya-Ju Song

We study the decoherence speed limit (DSL) of a single impurity atom dopped in a Bose-Einstein-condensed (BEC) reservoir when the impurity atom is in a double-well potential. We demonstrate how the DSL of the impurity atom can be manipulated by engineering the BEC reservoir and the impurity potential within experimentally realistic limits. We show that the DSL can be controlled by changing key parameters such as the condensate scattering length, the effective dimension of the BEC reservoir, and the spatial configuration of the double-well potential imposed on the impurity. We uncover the physical mechanisms of controlling the DSL at root of the spectral density of the BEC reservoir.

P-012

Excited States of Squaraines via Linear and Non-Linear Electronic Absorption

Freda Jean Mwasha

Squaraines are known to exhibit interesting photochemistry and large 2PA cross-sections, with potential application in photodynamic therapy (PDT). Through response functions (linear and quadratic), implemented in TD-DFT we investigate the spectra of one photon absorption (OPA), two-photon absorption (2PA) and excited state absorption (ESA) in a halogenated and unhalogenated squaraine. We also evoke the a posteriori Tamm-Danco approximation (ATDA) to determine 2PA cross sections without a quadratic response function, through a three-state model.

P-013

Tacticity Prediction of Poly(methyl methacrylate) from Radical Polymerization via Red Moon Methodology

Zizhen Rao

Ribulose-1,5-bisphosphate carboxylase/oxygenase, commonly known by the abbreviations “RuBisCO”, is an enzyme involved in the first major step of carbon fixation, a process by which atmospheric carbon dioxide is converted by plants and other photosynthetic organisms to energy-rich molecules such as glucose. It is well known that a kinetic isotope effect occurs in the carboxylation process. To describe the reaction, ONIOM-MD simulation has been employed. QM part of ONIOM model was determined as a region which contains Mg^{2+} ion, RuBP (Ribulose-1,5-bisphosphate), CO_2, Lys175, Lys177, Asp203, Glu204, His294, Lys334 and KCX201, refer to the “FM20” cluster model . A tunnel for CO_2 has been observed in MD simulation and assuming the reaction path from the inlet of CO_2 to the product through the coordinate complex by Mg^{2+}, the simulations have been performed on the several molecular configuration models with fixing the geometries between CO_2 and RuBP along the tunnel. Thus free energy for these models could be obtained to determine the reaction rate constant, k, from the velocity of the whole atoms from trajectories. Then the isotope effect $\alpha = k_{12CO2}/k_{13CO2}$ could be estimated by changing mass of carbon.

P-014

Neural Network Fitted Kinetic Energy Densities of Different Classes of Materials

Pavlo Golub

We explore neural network (NN) fits to kinetic energy densities (KED) of molecules and solids, including light metals and semiconductors for the purpose of producing machine-learned semi-local kinetic energy functionals (KEF) for orbital-free DFT. We use terms of the fourth-order gradient expansions of the kinetic energy density (KED) as density-dependent variables. The formal fourth-order expansion is convergent for periodic systems and small molecules but does not improve over the second-order expansion (Thomas-Fermi term plus one-ninth of von Weizsäcker term). Linear fitting of the expansion coefficients somewhat improves on the formal expansion. A much more accurate match with the Kohn-Sham KED is achieved by using NNs trained using the terms of the 4th order expansion as inputs. We obtain ultra-low fitting errors without overfitting. Small single hidden layer neural networks can provide good accuracy in separate KED fits of each compound, while for joint fitting of KEDs of multiple compounds multiple hidden layers were required to achieve good fit quality. The critical issue of data distribution is highlighted. We also show the critical role of pseudopotentials in the performance of the expansion, where in the case of a too rapid decay of the valence density at the nucleus with some pseudopotentials, numeric instabilities arise.

P-015

Non-Nuclear Attractors in Small Charged Lithium Clusters, Li_m^q (m = 2-5, q = ±1), with QTAIM and the Ehrenfest Force Partitioning

Alireza Azizi

In this investigation we explore the function and existence of the non-nuclear attractor (*NNA*) for a series of small charged lithium clusters Li_m^q (m = 2-5, q = ±1) using QTAIM and the Ehrenfest Force $\mathbf{F}(\mathbf{r})$ partitioning schemes. The *NNA*s were found to be present in all of the Li_m^q (m = 2-5, q = ±1) clusters for QTAIM, in contrast none were found for $\mathbf{F}(\mathbf{r})$. We discovered that the anionic and cationic lithium dimers are limiting cases for minimal and maximal impact of the *NNA* related to the relative sparseness of total charge density $\rho(\mathbf{r})$ distributions respectively. Evidence is found that the *NNA* in the anionic dimer is in the process of being annihilated by two neighboring *BCP*s. We provide a measure of the size of the *NNA* and find for Li_m^q (m = 2-5, q = ±1) that larger *NNA*s correlate with increased Li-Li separations. The *NNA* was determined to be a persistent feature by varying the Li separations for the cationic and anionic dimers. Very large Li separations failed to induce an *NNA* in the $\mathbf{F}(\mathbf{r})$ anionic dimer and therefore we conclude that $\mathbf{F}(\mathbf{r})$ is unable to detect *NNA*s. The metallicity $\xi(\mathbf{r}_\mathrm{b})$ was also used to measure the sparseness of the distribution of $\rho(\mathbf{r})$ and significant metallic character, on the basis of $\xi(\mathbf{r}_\mathrm{b}) > 1$, was present for QTAIM but not for $\mathbf{F}(\mathrm{r})$, providing further evidence that $\mathbf{F}(\mathbf{r})$ cannot detect *NNA*s. Advantages of the use of Ehrenfest Force $\mathbf{F}(\mathbf{r})$ partitioning scheme are discussed that include the design of nano-devices through tuning of the Ehrenfest potential $V_\mathrm{F}(\mathbf{r}\ \mathbf{b})$ by the application of external forces such as a constant electric or strain field.

P-015

A Vector-Based Representation of the Chemical Bond for Predicting Competitive and Non-Competitive Torquoselectivity of Thermal Ring-Opening Reactions

Alireza Azizi

We present a new vector-based representation of the chemical bond referred to as the bond-path frame-work set $\mathrm{B} = \{p, q, r\}$, where p, q and r represent three paths with corresponding eigenvector-following paths with lengths H^*, H and the bond-path length from the quantum theory of atoms in molecules (QTAIM). We find that longer path lengths H of the ring-opening bonds predict the preference for the transition state inward (TSIC) or transition state outward (TSOC) of thermal ring opening reactions in agreement with experiment for all five reactions **R1-R5**. Competitiveness and non-competitiveness have traditionally been considered using activation energies within transition state theory that is known to fail for thermal ring-opening reactions. Consequently, we find that the activation energy for **R3** does not satisfactorily determine competitiveness or provide consistent agreement with experimental yields. We choose a selection of five competitive and non-competitive reactions; methyl-cyclobutene (**R1**), ethyl-methyl-cyclobutene (**R2**), iso-propyl-methyl-cyclobutene (**R3**), ter-butyl-methyl-cyclobutene (**R4**) and phenyl-methyl-cyclobutene (**R5**). Therefore, in this investigation we provide a new criterion, within the QTAIM framework, to determine whether the reactions **R1-R5** are competitive or non-competitive. We that find **R2**, **R3** and **R5** are competitive and **R1** and **R4** are non-competitive reactions in contrast to the results from the activation energies, calling into question the reliability of activation energies

P-016

The Role of Weak Interactions in Characterizing Peptide Folding Preferences Using a QTAIM Interpretation of the Ramachandran Plot (ϕ-ψ)

Roya Momen

The original Ramachandran plot is a potent way to understand structures of biomolecules, however only backbone conformations are considered. We formulate a new interpretation of the original Ramachandran plot (ϕ-ψ) that can include a description of the weaker interactions including both the hydrogen bonds and H---H bonds as a new way to derive insights into the phenomenon of peptide folding. Specifically, we show that QTAIM analysis permits identifying key regions of the Ramachandran plot without the need for massive data sets. The QTAIM interpreted Ramachandran plot is derived from QTAIM eigenvectors and not a trivial coordinate transformation. An investigation of both the backbone and the weaker bonds within the framework of the QTAIM interpreted Ramachandran plot was found to be in line with physical intuition. The least-preferred directions calculated for the hydrogen bonds and H---H bonds were found to coincide with the “unlikely” regions of the Ramachandran plot.

P-017

Exploration of the Forbidden Regions of the Ramachandran Plot (ϕ-ψ) with QTAIM

Roya Momen

A new QTAIM interpretation of the Ramachandran plot is formulated from the most and least facile eigenvectors of the second-derivative matrix of the electron density with a set of 29 magainin-2 peptide conformers. The presence of QTAIM eigenvectors associated with the most and least preferred directions of electronic charge density explained the role of hydrogen bonding, H---H contacts, and glycine amino acid monomer in peptide folding. The highest degree of occupation of the QTAIM interpreted Ramachandran plot was found for the H--O/H---O and H---H bonds followed by the glycine amino acid monomer with the least occupation for the remaining backbone peptide bonds. The mobility of the QTAIM eigenvectors of the glycine amino acid monomer was higher than for the other amino acids and was comparable to that of the hydrogen bonding, explaining the flexibility of the magainin-2 backbone. We experimented with a variety of hybrid QTAIM-Ramachandran plots to highlight and explain the why the glycine amino acid monomer largely occupies the ‘forbidden’ on the Ramachandran plot. In addition, the new hybrid QTAIM-Ramachandran plots contained recognizable regions that can be associated with concepts familiar from the conventional Ramachandran plot whilst retaining the character of the QTAIM most and least preferred regions.

P-018

Next-Generation Quantum Theory of Atoms in Molecules for the Ground and Excited States of the Penta-2,4-dieniminium Cation (PSB3)

Xin Bin

A 3-D vector-based representation of the chemical bond recently introduced, the bond-path frame-work set B, is applied to analysis of the minimum energy pathways corresponding to deactivation of the first excited singlet state of PSB3 and occurring through torsion about the three double bonds of PSB3 combined with other intramolecular degrees of freedom, such as the bond length alternation. Using the bond-path framework set B analysis we elucidate the importance of a balanced treatment of the covalent and ionic contributions to the ground and excited state originating from torsion about various double bonds, which is known to be strongly dependent on the presence of dynamic electron correlation. Therefore, we present a more sophisticated method of determination of the degree of covalent and ionic contributions known to be responsible for altering the relative stability of the S_1/S_0 conical intersections. The presented results suggest that the commonly used simplified multi-reference methodologies that omit the dynamic correlation are to be avoided as they often result in incorrect predictions for the excited state deactivation reaction mechanism.

P-019

Next-Generation Quantum Theory of Atoms in Molecules for the Ground and Excited States of Fulvene

Weijie Huang

A new interpretation of the chemical bond that we refer to as the bond-path frame-work $\mathbb{B}$, is presented. By contrast to the usual bond-path of the conventional quantum theory of atoms in molecules (QTAIM), the new definition can differentiate between the ground and excited states of molecules. The new interpretative tool is applied to excited state deactivation of fulvene. The excited state deactivation of fulvene involves distortions along various intramolecular degrees of freedom, such as bond stretching/compression bond length alternation (BLA) and bond torsion distortions. For the BLA distortion and the torsion coordinate, three unique elements were obtained for $\mathbb{B}$.

P-020
A Vector-Based Representation of the Chemical Bond for the Normal Modes of Benzene
Weijie Huang

We introduce a vector-based interpretation of the chemical bond within the quantum theory of atoms in molecules (QTAIM), the bond-path framework set $\mathbb{B}$, to determine the participation of each of the C-H and C-C bonds of the four infra-red (IR) active normal modes of benzene. We the bond-path framework set $\mathbb{B}$ comprises three components, including eigenvector-following path lengths $\mathbb{H}^*$, $\mathbb{H}$ and the bond-path length (BPL) that is already familiar within QTAIM. The bond-path framework set $\mathbb{B}$ follows variations with amplitude along an entire bond-path, as opposed to only at the bond critical point (BCP), during a normal mode of vibration beyond purely geometrical considerations. In doing so we establish the presence of bond-path torsion that occurs during the amplitude vibration of the four IR active normal modes, without the need for either dihedral angles or reference directions. We find that the 3-D morphology in terms of bond stretching/compression and torsion of the four IR normal modes. We introduce a couple of fractional eigenvector-following path lengths $\mathbb{H}_f$ and $\mathbb{H}_{fmin}$ that can follow small variations more effectively than the analogous QTAIM bond-path curvature.

P-021
QTAIM and Stress Tensor Bond-path Framework Sets for the Ground and Excited States of Fulvene
Weijie Huang

We present, for the ground and first excited states of fulvene, the complete 3-D bond-path framework set $\mathbb{B} = \{(p_0,p_1), (q_0,q_1), (r_0,r_1)\}$ from the quantum theory of atoms in molecules (QTAIM) and $\mathbb{B}_{\sigma H} = \{(p_{\sigma H0},p_{\sigma H1}), (q_{\sigma H0},q_{\sigma H1}), (r_0,r_1)\}$ and $\mathbb{B}_\sigma = \{(p_{\sigma 0},p_{\sigma 1}), (q_{\sigma 0},q_{\sigma 1}), (r_0,r_1)\}$ from the stress tensor within the QTAIM partitioning. We find that both the QTAIM bond-path framework sets $\mathbb{B} = \{(p_0,p_1), (q_0,q_1), (r_0,r_1)\}$ and the stress tensor $\mathbb{B}_\sigma = \{(p_{\sigma 0},p_{\sigma 1}), (q_{\sigma 0},q_{\sigma 1}), (r_0,r_1)\}$ provide a quantitative 3-D rendering of the bonding that is consistent with understanding of the bonding provided by using Lewis structures.

P-022
The 3-D Bonding Morphology of the Infra-Red Active Normal Modes of Benzene
Weijie Huang

We present for the first time a visualization of the 3-D morphology of all the C-C and C-H bonds for the four infra-red (IR) active normal modes of benzene using the complete bond-path framework set $\mathbb{B} = \{\boldsymbol{p}, \boldsymbol{q}, \boldsymbol{r}\}$ a vector-based interpretation of the chemical bond within the QTAIM framework. The bond-path framework set $\mathbb{B} = \{\boldsymbol{p}, \boldsymbol{q}, \boldsymbol{r}\}$ comprises three strands in the ground state, with the ***r***-path corresponding to the familiar QTAIM concept of bond-path. The two new paths, the ***p***-path and ***q***-path are formulated from the least and most preferred directions of electron density accumulation respectively.

P-023
A Vector-Based Representation of the Chemical Bond for the Substituted Torsion of Biphenyl
Jiahui Li

We use a new interpretation of the chemical bond within QTAIM, the bond-path framework set $\mathbb{B} = \{\boldsymbol{p},\boldsymbol{q},\boldsymbol{r}\}$ with associated linkages with lengths $\mathbb{H}^*$, $\mathbb{H}$ and the familiar bond-path length is used to describe a torsion θ, $0.0° \leq \theta < 22.0°$ of *para*-substituted biphenyl, $C_{12}H_9$-*x*, *x* = $N(CH_3)_2$, NH_2, CH_3, CHO, CN, NO_2. We include consideration of the H---H bonding interactions and find that the lengths $\mathbb{H} > \mathbb{H}^*$ that we explain in terms of the most and least preferred directions of charge density accumulation. We also consider the fractional eigenvector-following path with lengths $\mathbb{H}_f$ and $\mathbb{H}_{f\theta min}$..

P-024

Stress Tensor Eigenvector Following with Next-Generation Quantum Theory of Atoms in Molecules

Jiahui Li

The eigenvectors of the electronic stress tensor have been identified as useful for the prediction of chemical reactivity because they determine the most preferred directions to move the bonds that correspond to a qualitative change in the molecular electronic structure. A new 3-D vector based interpretation of the chemical bond that we refer to as the bond-path framework set $\mathbb{B} = \{\boldsymbol{p},\boldsymbol{q},\boldsymbol{r}\}$ provides a version of the quantum theory of atoms in molecules (QTAIM) beyond the minimum definition for bonding that is particularly suitable for understanding changes in molecular electronic structure that occur during reactions. The bond-path framework set $\mathbb{B}$ is straightforwardly constructed and visualized from the eigenvalues and eigenvectors of QTAIM. This approach is applied to the structural deformations of ethene that occur during applied torsion θ, $-180.0\,° \leq \theta \leq +180.0\,°$. The corresponding stress tensor version is readily constructed as $\mathbb{B}_\sigma = \{\boldsymbol{p}_\sigma,\boldsymbol{q}_\sigma,\boldsymbol{r}\}$ within the QTAIM partitioning making it possible to compare experimentally and computationally determined electronic charge densities. The bond-path framework set $\mathbb{B}$ or $\mathbb{B}_\sigma$ are the networks that comprise three strands: the least preferred ($\boldsymbol{p}$,$\boldsymbol{p}_\sigma$), most preferred ($\boldsymbol{q}$,$\boldsymbol{q}_\sigma$) and $\boldsymbol{r}$ is the familiar QTAIM bond-path. We demonstrate that the most preferred direction for bond motion using the stress tensor corresponds to the most compressible direction and not to the least compressible direction as previously reported. We show the necessity for a directional approach constructed using the eigenvectors along the entire bond length and demonstrate the insufficiency of the sole use of scalar measures for capturing the nature of the stress tensor within the QTAIM partitioning.

P-025

Consequences of Theory Level Choice Evaluated with New Tools from QTAIM and the Stress Tensor for a Dipeptide Conformer

Jiahui Li

QTAIM and the stress tensor were used to provide a detailed analysis of the topology of the molecular graph, *BCP* and bond-path properties, including the new introduced helicity length $\mathbb{H}$, of a Tyr-Gly dipeptide conformer subjected to a torsion with four levels of theory; MP2, M06-2X, B3LYP-D3 and B3LYP and a modest-sized basis set, 6-31+G(d).

Structural effects and bonding properties are quantified and reflect differences in the BSSE and lack of inclusion of dispersion effects in the B3LYP calculations. The helicity length $\mathbb{H}$ demonstrated that MP2 produced a unique response to the torsion suggesting future use as a diagnostic tool.

P-026

Next-Generation Quantum Theory of Atoms in Molecules for the Ground and Excited State of the Ring-Opening of Cyclohexadiene (CHD)

Tian Tian

The factors underlying the experimentally observed branching ratio (70:30) of the (1,3-cyclohexadiene) CHD→HT (1,3,5-hexatriene) photochemical ring-opening reaction are investigated. The ring-opening reaction path is optimized by a high-level multi-reference DFT method and the density along the path is analyzed by the QTAIM and stress tensor methods. The performed density analysis suggests that, in both S_1 and S_0 electronic states, there exists an attractive interaction between the ends of the fissile σ-bond of CHD that steers the ring-opening reaction predominantly in the direction of restoration of the ring. It is suggested that opening of the ring and formation of the reaction product (HT) can only be achieved when there is a sufficient persistent nuclear momentum in the direction of stretching of the fissile bond. As this orientation of the nuclear momentum vector can be expected relatively rare during the dynamics, this explains the observed low quantum yield of the ring-opening reaction.

P-027

Consequences for Stereochemistry of Locating the Chirality-Helicity Equivalence in the S and R Stereoisomers of Lactic Acid

Tianlu Xu

We locate the missing chirality-helicity equivalence present for molecules with a chiral center and as a consequence the degeneracy of the S and R stereoisomers of lactic acid was lifted. Agreement was found with the naming schemes from the optical experiments from the most and least preferred directional preferences CCW (left-handed) and CW (right-handed) of the S and R stereoisomers respectively. We explain the consequences for stereochemistry in terms of the ability to determine the chirality of industrially relevant reaction products. This was made possible by the construction of the stress tensor trajectories $\mathbb{T}_\sigma(s)$ that comprise the necessary symmetry breaking by using a mapping from each bond critical point shift vector $\pm\mathbf{dr}$ in real space to a point in $\mathbb{U}_\sigma$ space. This was undertaken by applying a symmetry breaking torsion θ, $-180.0\,° \leq \theta \leq +180.0\,°$ corresponding to clockwise (CW) and counter-clockwise (CCW) directions. We explain why the bond ellipticity ε from the Quantum Theory of Atoms in Molecules is able to lift the degeneracy everywhere except θ = 0.0°, ±60.0°, ±120.0° and ±180.0° corresponding to the extrema in the relative energy ΔE and yields a mirror image for the rotational isomers of the S and R stereoisomers.

P-028
Relativistic motion enhanced quantum estimation of κ-deformation of spacetime
Xiaobao Liu

We probe the κ-deformation of spacetime using a two-level atom as a detector coupled to a κ-deformed mass-less scalar field which is invariant under a κ-Poincaré algebra and written in commutative spacetime. To address the quantum bound to the estimability of the deformation parameter κ, we perform measurements on the two-level detector and maximize the value of quantum Fisher information over all possible detector preparations. We prove that the population measurement is the optimal measurement in the estimation of the deformation parameter κ. In particular, we show that the relativistic motion of the detector affects the precision in the estimation of the parameter κ, which can effectively improve this precision comparing to that of the static detector case by many orders of magnitude.

P-029
Strong exciton-photon coupling in solution grown CsPbBr3 micro/nanowires
Zhuang Zhao

Cesium lead halide perovskites have attracted people's attention with its high performance and stability. Recently the all-inorganic perovskite nanowires have drawn considerable attention for the important applications in optoelectronic devices with its stronger photon confinement. What’s more, in the strong light-matter interaction region, their high exciton oscillation intensity and binding energy make them so important for polariton devices. In this work, we report an easy way to get the high-quality CsPbBr3 nanowire by synthesizing in solution. By means of studying the CsPbBr3 spatial resolved PL spectra, we observed long and strong exciton-photon coupling after the main peak (527nm).Moreover, by changing the laser excitation power and temperature, we proved the presence of the particular high vacuum Rabi splitting energy and the formed exction-polaritons. All these results present the strong exciton-photon coupling in solution grown all-inorganic CsPbBr3 micro/nanowire at room temperature. Our results are significant for the development of high performance and stability polariton-based incoherent and coherent sources and give the new way to promote the light applications. More importantly establishing the foundation of the large-scale application.

P-030
Surface polarons and optical micro-cavity modulated broad range multi-mode emission of Te-doped CdS nanowires
Qi Zheng

As a result of the low dimensionality and native optical resonator, one-dimensional (1D) semiconductor nanostructures offer a critical platform to study the confined coherent transport of phonons, photons, electrons, excitons and polarons etc along a definite direction. we synthesized highquality hexagonal Te-doped CdS nanowires by two-step chemical vapor deposition and investigated systematically the doping concentration, temperature, excitation power, excitation wavelength dependent Raman, photoluminescence and carrier lifetime decay. The strong surface optical (SO) phonon mode is observed in the micro-Raman spectra of an individual Te–CdS nanowire, which is unsuitable in large-sized structures. In situ micro-photoluminescence (μ-PL) characterization shows dominant confined defect state emission with whispering gallery mode (WGM) characteristics. The emission peak position shifts under increased excitation power, demonstrating the inelastic scattering by bound carriers. In addition, the short wavelength emission modes are dominant at a low temperature (80 K) while the long wavelength emission modes are dominant at a high temperature (300 K) due to different recombination processes contributing to the WGM resonant bands, which was also confirmed by the time-resolved PL measurement. All these results reflect strong coupling between the surface evanescent-wave in the WGM cavity and the SO phonon/polaron, which will facilitate the rational tailoring of surface/interface relevant properties for nanophotonic device applications.

P-031
The preferred slip plane of nuclear material of Hafnium: A first-principles study
Heyu Zhu

In this work, first-principles calculations based on density functional theory (DFT) were applied to simulate the general stacking faults energy (GSFE) of all the possible basal, prism and pyramidal planes of Hafnium (Hf), which was applied as an ideal neutron absorber in nuclear industry. The calculations reveal that unlike titanium (Ti) and zirconium (Zr) having preferred slip plane of prism, the same group of Hf has lower GSFE in basal plane (I2) than that in prism plane (SF1), i.e., the preferred slip plane of Hf is basal rather than prism. Our prediction well meets the recent experimental result. In order to ensure the precise of the stacking faults energy calculations, in-plane and out-of-plane directions of relaxations were considered in detail. For basal and prism plane, the effect from in-plane direction relaxation on GSFE was eligible, while for pyramidal plane, both in-plane and out-of-plane directions of relaxations should be included in the calculations.

P-032
Photon blockade effect in a coupled cavity system
Fen Zou

We study the photon blockade effect in a coupled cavity system, which is formed by a linear cavity coupled to a Kerr-type nonlinear cavity via a photon-hopping interaction. We explain the physical phenomenon from the viewpoint of the conventional and unconventional photon blockade effects. The corresponding physical mechanisms of these two photon blockade effects are based on the anharmonicity in eigenenergy spectrum and the destructive quantum interference between two different transition paths, respectively. In particular, we find that the quantum interference effect also exists in the conventional photon blockade regime. Our results are confirmed by analytically and numerically solving the quantum master equation and calculating the second-order correlation function of the cavity fields. This model is general and hence it can be implemented in various experimental setups such as coupled optical cavity systems, coupled photon-magnon systems, and coupled superconducting-resonator systems. We present some discussions on the experimental implementation.

P-033
Amorphous Co-Pi anchored on TiO_2/CdSe nanowire arrays for efficient photoelectrochemical hydrogen production
Cao Zhou

Photoelectrochemical (PEC) water splitting into hydrogen and oxygen using hybridized semiconductor photoelectrodes and electrocatalysts has become a promising strategy for converting solar energy into clean and sustainable H_2 fuel. However, most of the photoelectrodes have the critical issues of a poor efficiency and stability for practical PEC water splitting systems. Here we report a promising hybrid photoanode constructed by electrodepositing an amorphous Co-Pi film onto semiconducting TiO_2/CdSe nanowire arrays for oxygen evolution in water splitting. This photoanode exhibits a high water-splitting photocurrent density, which is attributed to the broad visible light absorption and efficient charge carrier separation by the virtue of the Type II heterojunction formed between TiO_2 and CdSe. The photo-conversion efficiency of this photoanode is greatly improved, which is more than three times relative to that of the pristine TiO_2 photoanode. In particular, electrodeposition of an amorphous Co-Pi film on top can endow the photoanode with a better PEC stability compared with the bare TiO_2/CdSe electrode, probably because of the addition of the Co-Pi film protecting the light absorber TiO_2/CdSe from photocorrosion.

P-034
The effect of alloying on the band engineering of two-dimensional transition metal dichalcogenides
Jiansheng Dong

We present a quantitative study to address a deeper insight on the relationship between the bond identities and band shift based on the atomic-bond-relaxation (ABR) correlation mechanism and valance-force-field (VFF) approach. We find the interaction parameter in 2D-TMDs alloys could be obtained from the lattice distortion energy and further reveal the bowing mechanism of composition tunable bandgap in 2D-TMDs.

P-035
Concurrence of Two Atoms in a Rectangular Waveguide：Linear Approximation
Lijuan Hu

We study the entanglement of two two-level atoms which is weakly coupled with a infinite long waveguide of rectangular cross section with area A=ab (a=2b) . The two atoms are separately fixed by a distance R.We found that when the interatomic distance is half wavelength,the spontaneous emission of atoms is effectively suppressed and then the concurrence can last a period of time.While the distance is quarter wavelength, the pair performs a cooperative behavior.

P-036
Nonlinear optomechanics with gain and loss: amplifying higher-order sideband and group delay Spectroscopy of Atoms and Ions
Yafeng Jiao

We study the nonlinear optomechanically induced transparency (OMIT) with gain and loss. We find that (i) for a single active cavity, significant enhancement can be achieved for the higher-order sidebands, including the transmission rate and the group delay; (ii) for active–passive-coupled cavities, hundreds of microsecond of optical delay or advance are attainable for the nonlinear sideband pulses in the parity-time-symmetric regime. The active higher-order OMIT effects, as firstly revealed here, open up the way to make a low-power optomechaical amplifier, which can amplify both the strength and group delay of not only the probe light but also its higher-order sidebands.

P-037

Controlling chaotic spin-motion entanglement of ultracold atoms via spin-orbit coupling *Olga Yu.*

Chao Kong

We study the spatially chaoticity-dependent spin-motion entanglement of a spin-orbit (SO) coupled Bose-Einstein condensate with a source of ultracold atoms held in an optical superlattice. In the case of phase synchronization, we analytically demonstrate that (a) the SO coupling (SOC) leads to the generation of spin-motion entanglement; (b) the area of the high-chaoticity parameter region inversely relates to the SOC strength which renormalizes the chemical potential; and (c) the highchaoticity is associated with the lower chemical potential and the larger ratio of the short-lattice depth to the longer-lattice depth. Then, we numerically generate the Poincare sections to pinpoint that the chaos probability is enhanced with the decrease in the SOC strength and/or the spindependent current components. The existence of chaos is confirmed by computing the corresponding largest Lyapunov exponents. For an appropriate lattice depth ratio, the complete stop of one of (or both) the current components is related to the full chaoticity. The results mean that the weak SOC and/or the small current components can enhance the chaoticity. Based on the insensitivity of chaos probability to initial conditions, we propose a feasible scheme to manipulate the ensemble of chaotic spin-motion entangled states, which may be useful in coherent atom optics with chaotic atom transport.

P-038

Simultaneous cooling of coupled mechanical resonators in cavity optomechanics

Denggao Lai

Quantum manipulation of coupled mechanical resonators has become an important research topic in optomechanics because these systems can be used to study the quantum coherence effects involving multiple mechanical modes. A prerequisite for observing macroscopic mechanical coherence is to cool the mechanical resonators to their ground state. Here we propose a theoretical scheme to cool two coupled mechanical resonators by introducing an optomechanical interface. The final mean phonon numbers in the two mechanical resonators are calculated exactly and the results show that the ground-state cooling is achievable in the resolved-sideband regime and under the optimal driving. By adiabatically eliminating the cavity field in the large-decay regime, we obtain analytical results of the cooling limits, which show the smallest achievable phonon numbers and the parameter conditions under which the optimal cooling is achieved. Finally, the scheme is extended to the cooling of a chain of coupled mechanical resonators.

P-039

Soft X-ray activated $NaYF_4$: Gd/Tb scintillating nanorods for in vivo dual-modal X-ray/ X-rayinduced optical bioimaging

Xiaolong Li

Lanthanide (Ln) nanocrystals using soft X-ray as an excitation source have received significant research interest due to the advantages of unlimited penetration depth of X-ray light. In this study, we demonstrated an efficient scintillator based on $NaYF_4$:Gd nanorods (denoted as NRs) doped with different contents of terbium (Tb) ions for optical bioimaging under X-ray irradiation. The experimental results showed that the emission intensity was correlated to the doping contents of Tb^{3+}, and the largest emission intensity was achieved by doping 15% Tb under excitation by soft X-ray light. In addition, the emission intensity of the as-prepared NRs can be significantly improved by increasing the excitation power and irradiation times of the X-ray. Owing to the efficient X-ray-induced emission, these NRs were successfully used as probes for X-ray-induced optical bioimaging with high sensitivity. In addition, the dual-modal X-ray imaging and X-ray induced optical bioimaging were performed on a mouse, which indicated that the NRs were promising dual-modal bioprobes. Therefore, the X-ray activation nature of the designed NRs makes them promising probes for biomedicine and X-ray-induced photodynamic therapy (PDT) applications owing to the unlimited penetration depth of X-ray excitation source and absence of autofluorescence.

P-040

Collapse and revival of quantum entanglement in a microscopic-macroscopic system consisting of two Rydberg impurities and a Bose-Einstein condensate

Zhen Li

We study dynamics of quantum entanglement in a Bose-Einstein condensate (BEC) system with two Rydberg impurities, which is a microscopic-macroscopic system which consists of two microscopic impurities and one macroscopic BEC. It is found that the impurities-dopped BEC system exhibits not only microscopic entanglement collapse and revival (ECR) between two Rydberg impurities, but also microscopic-macroscopic ECR between two Rydberg impurities and the BEC. We point out the possibility of controlling the ECR through changing key parameters of the impurities-dopped BEC system such as initial-state parameters and Rydberg impurities-BEC coupling strength, and uncover the physical mechanism behind the ECR phenonmenon. We show that the ECR can transfer from the two Rydberg impurities into two impurities and the BEC. We demonstrate that micro-entanglement between two impurities can perfectly transfer into the micro-macro entanglement between the BEC and two impurities. It is shown that there exists a curious complementarity between the micro-entanglement and the micro-macro entanglement. It is indicated that the BEC decoherence suppresses the entanglement revivals.

P-041

Symmetrical metallic and magnetic edge states of monolayer 1T-PtX2(X=S、Se)

Shan Liu

Transition metal dichalcogenides (TMD) MoS2 or graphene could be designed to metallic nanoribbons, which always have only one edge show metallic properties due to symmetric protection. In present work, a nanoribbon with two parallel metallic and magnetic edges was designed from a noble TMD PtS2 by employing first-principles calculations based on density functional theory (DFT). The band structure, density of states (DOS) and simulated scanning tunneling microscopy (STM) of three possible zigzag edge states of monolayer semiconductive PtX2 were systematically studied. Detailed calculations show that Pt-terminated edge state among three zigzag edge states was metallic. The Pt-terminated edge state designed from monolayer PtS2 show both metallic and magnetic properties.

P-042

Fringe visibility and distinguishability in two-path interferometer with an asymmetric beam splitter

Yanjun Liu

We obtain the fringe visibility and the distinguishability in a general Mach-Zehnder interferometer with an asymmetric beam splitter. Both the fringe visibility V and the distinguishability D are affected by the input state of the particle characterized by the Bloch vector S=（Sx,Sy,Sz）and the second asymmetric beam splitter characterized by paramter β. For the total system initially in a pure state, it is found that the fringe visibility reaches the upper bound and the distinguishability reaches the lower bound when cosβ = −Sx. The complementaryrelationship V2+ D2≤ 1 is proved to be established in a general MZI with an asymmetric BS.

P-043

Nonlinear Dicke Quantum Phase Transition and Its Quantum Witness in a Cavity-Bose–Einstein-Condensate System

Wangjun Lu

We investigate nonlinear Dicke quantum phase transition (QPT) induced by inter-atomic nonlinear interaction and its quantum witness in a cavity-Bose–Einstein-condensate (BEC) system. It is shown that inter-atomic nonlinear interaction in a cavity BEC system can induce first-order Dicke QPT. It is found that this nonlinear Dicke QPT can happen in an arbitrary coupling regime of the cavity and atoms. It is demonstrated that the quantum speed limit time can witness the Dicke QPT through its sudden change at the critic point of the QPT.

P-044

Negative Poisson's ratio in monolayer blue phosphorene nanoribbon with edge sulfur passivation

Yi Ren

Motivated by the recent successful growth of monolayer blue phosphorus (BlueP), here we study the mechanical property in connection with microstructure for zigzag BlueP nanoribbons (zBluePNRs) with different edge chemical modification. Based on the first-principles calculations, strikingly, we find that a narrow zBluePNR (~2 nm) with edge sulfur (S) passivation under an uniaxial tensile strain exhibit an important effect of negative Poisson’s ratio because of the particularity of the P-S bonds at edges, and as the ribbon width increases the Poisson’s ratio varies from negative to positive. Meanwhile, the S-passivation also induces magnetism, and applying a strong enough strain can transfer a zBluePNR from magnetic metal state to half-metal one.

P-045

Sensitivity enhanced refractive index sensor by reducing the influence of in-plane wavevector in photonic spin Hall effect

Lijuan Sheng

Photonic spin Hall effect (SHE) can be an effective sensor for determining the refractive index (RI) variation of sensing medium. How to further improve its sensitivity is a very interesting and important issue. In this paper, we theoretically propose a weak measurement method for enhancing the sensitivity of the photonic SHE based RI sensor by reducing the influence of the in-plane wavevector. Of particular interest, our results indicate that the sensitivity of the presented configuration reaches about 3.16×10-7 RIU/μm which shows nearly two orders of magnitude improvement compared with the conventional one. Remarkably, this method can be applied for wide range of RI variation of sensing medium while keeping the high sensitivity.

P-046

Effect of In doping on the topological surface states of Bi2Se3

Ao Zhang

We investigate the effects of In doping on the topological surface states of Bi2Se3 based on first-principals calculations. We model the doping of In by replacing a Bi underneath the surface Se in supercells of five quintuple layer (5 QL) Bi2Se3. The doping of In tends to enlarge the distance between the surface QL and the sub-QL. Unfolded band structure were obtained by projecting the wavefunctions of the supercells on to the k- points in the Brillouin zone of the 1×1 unit cell of Bi2Se3 to reveal the effects of doping In on the band structure of Bi2Se3 thin film. We find that the doping of In results in a gaped band structure with Rashba-like splittings instead of Dirac cone. Layer-projection reveals that the splittings do not have the Rashba origin, but rather a relative shift of the Dirac cone for the two surface. Such a shift is due to the asymmetry potential caused by In doping. Consequently, the Klein tunneling induces gap openings for states away from the Γ point, while the Dirac states are somehow preserved. By the surface local density of states (LDOS), we find that In doping leads to loss of the weight of Dirac states.

P-047

Geometrical effect of thermal conductivity in 2D silicon flms with periodic nanopores

Liang Zhang

The thermal conductivity (TC) of periodic np-SiFs was investigated in relation to their geometric in terms of the atomic-bond-relaxation correlation mechanism and continuous medium mechanics by using the phonon kinetic method with the Born–von Karman dispersion relation. It was found that the 2D np-SiFs have high surface-to-volume ratios and elastic interactions among nanopores, which will change the Debye temperature, modify the phonon dispersion relation, reduce phonon group velocity, and further lead to the reduction of TC.

P-048

Band Modulation of Black Phosphorus and Molybdenum Disulfide Van Der Waals Heterojunction: Twist and Electric Field Effects

Zhe Zhang

The understanding of band modulation and related band alignment in van der Waals heterojunctions (vdW HJs) is of great importance to their electronic properties and potential applications in the field of nanoelectronic devices. In our work, we investigate the band evolusion and band alignment of black phosphorus (BP) and molybdenum disulfide (MoS_2) vdW HJs under the approaches of twist and applied electric field using first-principles calculations. It is founded that the positions and orbital contributions of conduction band minimum (CBM) and valence band maximum (VBM) in bilayer BP/MoS_2 HJs will alter as the composition twists relative to each other, while the major orbital contributions that are d_{z^2} states of Mo atoms and p_z states of P atoms do not change. When applying an electric field, the bilayer BP/MoS_2 HJs can experience type-II/I/II, indirect/direct/indirect bandgap, and semiconductor/metal transformations, respectively. The underlying mechanism on the twist effect and electric field modulation of electronic properties in BP/MoS_2 HJs has been clarified in detail. Our results show the essential information for the band engineering of BP/MoS_2 HJ and future device fabrication.

. P-049

Non-invasive through-skull brain vascular imaging and small tumor diagnosis based on NIR-II emissive lanthanide nanoprobes beyond 1500 nm

Zhenluan Xue

Optical bioimaging by using the new short-wavelength infrared window (SWIR, also named as NIR-II, 1000e1700 nm) is emerged as a next generation imaging technique for disease diagnosis owing to the unprecedented improvements in imaging sensitivity and spatial resolution. However, it is challenging to search new imaging agents with highly biocompatible and bright narrow-band emission located in the 1500e1700 nm (referred as NIR-IIb) region. Here we developed high quality polyacrylic acid (PAA) modified NaYF4:Gd/Yb/Er nanorods (PAA-NRs) with remarkably enhanced NIR-IIb emission and decent bio-compatibility for in vivo cerebral vascular bioimaging and small tumor visualization. These PAA-NRs present efficient narrow-band NIR-IIb emission centered at 1520 with 182 nm of band-width. Owing to the highly efficient NIR-IIb emission, NIR-IIb imaging-guided small tumor (4mm in diameter) detection is achieved. More importantly, non-invasive optical brain vessel bioimaging with high spatial (~43.65 mm) and temporal resolution through scalp and skull is obtained without craniotomy. These findings open up the opportunity of designing non-invasive approach for visualization the brain vasculature and tumor in biomedical application.

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