QSCP

XXII
2017
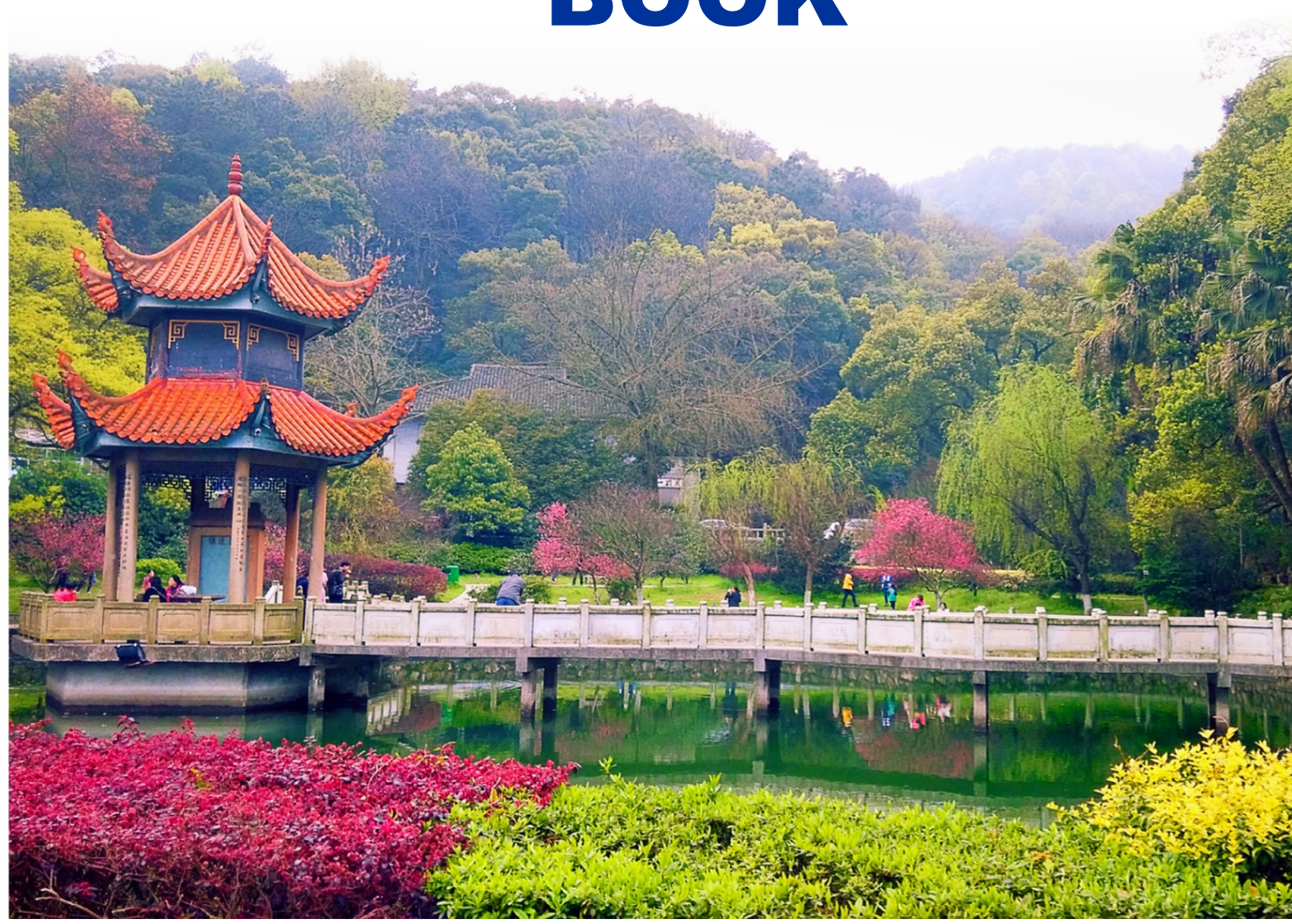
XXII International Workshop on

Quantum Systems in Chemistry, Physics and Biology

Changsha,China. OCTOBER 16-21, 2017.
http://www.qscp2017.org/

PROGRAM
BOOK

Twenty-Second International Workshop on Quantum Systems in Chemistry, Physics and Biology (QSCP-XXII)

October 16-21, 2017

Changsha, China

Scientific programs arranged by day

Arrangement of the Conference

The Timing and Location of the Conference

- 16th, Oct. 17:00-17:30 Opening Ceremony: Hunan Room III, 4th Floor in Main Building
- 16th, Oct. 17:45-19:15 Plenary Talks: Hunan Room III, 4th Floor in Main Building
- 17th - 21th, Oct. Keynote/Invited Talks: Hunan Room III, 4th Floor in Main Building
- 18th, Oct. Keynote/Invited Talks (Parallel Session): Changsha Room, 4th Floor in Main Building
- 20th, Oct. 19:00 Poster Session: along the corridor outside of Hunan Room III, 4th Floor in Main Building

Dining Room of the Conference

- 16th, Oct. 19:15 - 20:15 Welcome Reception: Sense Café, 2nd Floor in Main Building
- 19th, Oct. 18:00 - 20:00 Banquet and CMOA Award ceremony: Hunan Room II, 4th Floor in Main Building
- 16th - 21th, Oct. Lunch and Dinner: Sense Café, 2nd Floor in Main Building

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Opening Ceremony

Monday, 16 October P.M   Hunan Room III

Chaired by Samantha Jenkins

17:00 to 17:30
> Chair's speech:
> **Jean Maruani** (Chair of the QSCP International Scientific Committee)
> Welcome speech:
> **Hongxin Jiang** (President of Hunan Normal University)

17:30 to 17:45
> Take a conference photo (Front Square of the Hotel)

Plenary Talks

Monday, 16 October P.M   Hunan Room III

Chaired by Frank E. Harris

17:45 to 18:30
> **Rudolph A. Marcus** (California Institute of Technology, California, USA)
> **Reaction rate-thermodynamic relations and application to single molecule experiments on a biomolecular motor, F_1-ATPase**

18:30 to 19:15
> **Kwang S. Kim** (Ulsan National Institute of Science and Technology, Ulsan, South Korea)
> **Interplay between theory & experiment towards novel optics/ electronics/spintronics and efficient energy conversion**

Welcome Reception

Monday, 16 October P.M   Sense Café

19:15 to 20:15
> Self-service Dinner

Keynote/Invited Talks

Tuesday, 17 October A.M   Hunan Room III

Chaired by Kwang Soo Kim

09:15 to 09:50

Alain Dubois (Université Pierre et Marie Curie – CNRS, France)
Electronic processes in Cq^+-He, H collisions of relevance for fusion plasmas

09:50 to 10:15

Artur F. Izmaylov (University of Toronto, Scarborough, Canada)
Fully quantum non-adiabatic dynamics in the adiabatic representation

10:15 to 10:40

Ming Lei (Beijing University of Chemical Technology)
Metal-Substrate Cooperation Mechanism for Dehydrogenative Amidation Reaction Catalyzed by a PNN-Ru Catalyst

Chaired by Yasuteru Shigeta

11:00 to 11:35

Erkki J. Brändas (Uppsala University, Uppsala, Sweden)
Communication Simpliciter: Darwinian Evolution Reconsidered

11:35 to 12:00

Xiongjun Liu (Peking University, Beijing, China)
Observe spin-orbit coupling and topological physics for ultracold atoms

12:00 to 12:25

Anlian Pan (Hunan University, Changsha, China)
Band Gap and Interface Engineering of Low Dimensional Semiconductor Heterostructures

Keynote/Invited Talks

Tuesday, 17 October P.M   Hunan Room III

Chaired by Alain Dubois

14:00 to 14:25
> **Jeng-Da Chai** (National Taiwan University, Taiwan)
> Recent Advances in Thermally-Assisted-Occupation Density Functional Theory (TAO-DFT)

14:25 to 14:50
> **Pradeep R. Varadwaj** (The University of Tokyo, Tokyo, Japan)
> Halde Perovskite Solar Cell Semiconductors: A Perspective On Their Bonding Scenarios

14:50 to 15:15
> **Kaito Takahashi** (Academia Sinica, Taipei, Taiwan)
> Theoretical study on Criegee intermediate decay processes

Chaired by Kaito Takahashi

15:45 to 16:10
> **Yasuteru Shigeta** (University of Tsukuba, Tsukuba, Japan)
> An Enhanced Sampling Method for Searching Conformational Changes of Proteins and Supramolecules

16:10 to 16:35
> **Mengjie Wang** (Hunan Normal University, Changsha, China)
> Hawking Radiation for a Proca field

16:35 to 17:00
> **Yi Zhao** (Xiamen University, Xiamen, China)
> Time-dependent wave-packet diffusive method and its applications to Carrier quantum dynamics in organic materials

Keynote/Invited Talks

Wednesday, 18 October A.M   Hunan Room III

Chaired by Chao-Ping Hsu

09:00 to 09:25

Yibo Lei (Northwest University, Xi'an, China)
New Implementation of Static-Dynamic-Static second order perturbation theory (SDSPT2)

09:25 to 09:50

Paul A. Johnson (Université Laval, Quebec, Canada)
Model Wavefunctions for Strongly-correlated systems

09:50 to 10:15

Tanja van Mourik (University of St Andrews, St. Andrews, U.K)
On the mutagenicity of 5-bromouracil: Is tautomerism to blame?

Chaired by Erkki J. Brändas

11:00 to 11:25

Jianxin Song (Hunan Normal University, Changsha, China)
Synthetic Chemistry of Porphyrin Arrays and Porphyrinoids

11:25 to 11:50

Youwen Long (Institute of Physics, Chinese Academy of Sciences, Beijing, China)
Novel Magnetoelectric Multiferroicity in A-site Ordered Cubic Perovskite Oxides

11:50 to 12:15

Jun-ya Hasegawa (Hokkaido University, Hokkaido, Japan)
Constraint Structure Optimization for Minimum Energy Intersystem Crossing Point

Keynote/Invited Talks

Wednesday, 18 October A.M (Parallel)   Changsha Room

Chaired by Alia V. Tadjer

09:00 to 09:25
> **Michael Filatov** (Hunan Normal University, Changsha, China)
> Ensemble Density Functional Theory Method for Modeling Dynamics of Excited States

09:25 to 09:50
> **Xiao He**
> Interaction Entropy for Binding Free Energy

09:50 to 10:15
> **Ruibo Wu** ((Sun Yat-sen University, Guangzhou, China)
> Theoretical Studies on Terpenoids Biogenesis

Chaired by Masataka Nagaoka

11:00 to 11:25
> **Jian Liu** (Peking University, Beijing, China)
> A unified theoretical framework for mapping models for the multi-state Hamiltonian and a unified thermostat scheme for efficient configurational sampling

11:25 to 11:50
> **Qiang Zhao** (Institute of High Energy Physics, Chinese Acadamy of Sciences, Beijing, China)
> Exotic hadrons near threshold

Keynote/Invited Talks

Wednesday, 18 October P.M   Hunan Room III

Chaired by Wenjian Liu

14:00 to 14:25

> **Congzhang Gao**
> Towards the inclusion of dissipation in quantum time dependent, mean field theories

14:25 to 14:50

> **Herbert A. Früchtl** (University of St Andrews, St. Andrews, U.K)
> Quinone based building blocks for molecular electronics

14:50 to 15:15

> **Georgi V. Vayssilov** (University of Sofia, Sofia, Bulgaria)
> Elucidation of the Structure and Properties of Surface Species on Ceria Catalysts by Quantum Chemical Modeling

Chaired by Artur F. Izmaylov

15:45 to 16:10

> **Dahbia Talbi** (University of Montpellier, Montpellier, France)
> Theoretical chemistry for space chemistry

16:10 to 16:35

> **Xin Xu** (Fudan University, Shanghai, China)
> A fifth rung density functional that correctly describes both density and energy

16:35 to 17:00

> **Ling Xu** (Hunan Normal University, Changsha, China)
> Synthesis and Reactivity of Lutetacyclopentadiene

WEDNESDAY

Keynote/Invited Talks

Wednesday, 18 October P.M (Parallel)   Changsha Room

Chaired by Hongrong Liu

14:00 to 14:25
> **Mingxing Chen** (Hunan Normal University, Changsha, China)
> Giant Rashba spin splitting in supported stanene

14:25 to 14:50
> **Peng Zhang** (Renmin University of China, Beijing, China)
> Center of Mass Momentum Dependent Interaction Between Ultracold
> Atoms

Chaired by Youwen Long

15:45 to 16:10
> **Nike Dattani** (McMaster University, Hamilton, Canada)
> Computer Spectrometers!

16:10 to 16:35
> **Jieqiao Liao** (Hunan Normal University, Changsha, China)
> Macroscopic Quantum Superposition in Cavity Optomechanics

16:35 to 17:00
> **Hui Jing** (Hunan Normal University, Changsha, China)
> Defect-induced exceptional point in phonon lasing

Keynote/Invited Talks

Thursday, 19 October A.M   Hunan Room III

Chaired by Eberhard K. U. Gross

08:50 to 09:25
> **Nadine Halberstadt** (Universite Toulouse, Toulouse, France)
> Real time excited state dynamics of alkali-doped helium nanodroplets: A TDDFT study

09:25 to 09:50
> **Stijn Fias** (McMaster University, Hamilton, Canada)
> Chemical Transferability of Functional Groups Follows From the Nearsightedness of Electronic Matter

09:50 to 10:15
> **Mang Feng** (Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan, China)
> Exploring a new Heisenberg's error-disturbance relation using trapped ultracold ion system

10:15 to 10:40
> **James Anderson** (The University of Tokyo, Japan)
> Formulation of QTAIM for 2-Component Relativistic Hamiltonians

Chaired by Michael Filatov

11:00 to 11:35
> **Debashis Mukherjee** (Indian Association for the Cultivation of Science, Kolkata, India)
> Unitary Group Adapted Multi-reference Theories: State Universal and State Specific Approaches

11:35 to 12:00
> **Shinkoh Nanbu** (University of Sophia, Tokyo, Japan)
> Non-adiabatic *ab initio* Molecular Dynamics simulations in solution

12:00 to 12:25
> **Hui Dong** (Graduate School of Chinese Academy of Engineering Physics, Beijing, China)
> Berry curvature as a lower bound for multiparameter estimation

THURSDAY

Keynote/Invited Talks

Thursday, 19 October P.M   Hunan Room III

Chaired by Shinkoh Nanbu

14:00 to 14:35

Alia V. Tadjer (University of Sofia, Sofia, Bulgaria)
Design of TADF-Utilizing OLEDs

14:35 to 15:00

Masataka Nagaoka (Nagoya University, Nagoya, Japan)
Toward Controlling Complex Chemical Reactions in the Molecular
Aggregation States -From Multiscale Simulation to Computational
Molecular Technology

15:00 to 15:25

Samantha Jenkins (Hunan Normal University, Changsha, China)
Developments in QTAIM and Stress Tensor Theory

Chaired by Nadine Halberstadt

15:45 to 16:20

Chao-Ping Hsu (Academia Sinica, Taiwan)
Electronic coupling and rates for Singlet Fission

16:20 to 16:45

Su Yi (Institute of Theoretical Physics, Chinese Academy of Sciences,
Beijing, China)
Heisenberg-scaled magnetometer with dipolar spin-1 condensates

THURSDAY

Banquet and CMOA Award Ceremony

Thursday, 19 October P.M   Hunan Room II

18:00 to 18:30

Traditional Chinese Musical Performance

18:30 to 22:00

Banquet and CMOA Award Ceremony

Keynote/Invited Talks

Friday, 20 October A.M   Hunan Room III

Chaired by Akitomo Tachibana

09:00 to 09:25

Chaohong Lee (Sun Yat-sen University, Guangzhou, China)
Topological states and cotranslational symmetry in strongly interacting systems

09:25 to 09:50

Zhihui Peng (Hunan Normal University, Changsha, China)
Strong coupling between a cavity and a half open space via a superconducting artificial atom

09:50 to 10:15

Sol M. Mejía (Pontificia Universidad Javeriana, Bogotá, Colombia)
Molecular Characterization of
(Oligothiophene)n- tetracyanoquinodimethane complexes (n = 1-5)

Chaired by Jean Maruani

11:00 to 11:35

Wenjian Liu (Peking University, Beijing, China)
New Scenarios for Strongly Correlated Electrons

11:35 to 12:00

Rongzhen Liao (Huazhong University of Science and Technology, China)
QM and QM/MM Studies of Enzymatic Reactions: Mechanism and Selectivity

Keynote/Invited Talks

Friday, 20 October P.M   Hunan Room III

Chaired by Samantha Jenkins

14:00 to 14:35
> **Jean Maruani** (CMOA, France)
> The Dirac electron: physical consequences of deviations from whole numbers of the gyromagnetic factor, fine-structure constant, and gravitational invariant

14:35 to 15:00
> **Jun Li** (Tsinghua University, Beijing, China)
> Relativity-Induced Bonding Picture Change in Heavy-Element Compounds

15:00 to 15:25
> **Cristina E Gonzalez Espinoza** (McMaster University, Hamilton, Canada)
> Basis-set convergence in calculations with smooth Coulomb potentials

Chaired by Jianxin Song

15:45 to 16:20
> **Eberhard K. U. Gross** (Max Planck Institute of Microstructure Physics, Halle (Saale), Germany)
> Potential Energy Surfaces and Berry Phases beyond the Born-Oppenheimer Approximation: A New Perspective on Non-Aadiabatic Dynamics

16:20 to 16:45
> **Xinhua Peng** (University of Science and Technology of China, Beijing, China)
> Towards exotic quantum many-body physics on quantum simulator: Experimentally probing topological order and its breakdown

16:45 to 17:10
> **Wei Zhang** (Hunan Normal University, Changsha, China)
> Rational Construction of Organic Composite Microwire/Microdisk Hetero-structures for Controlled Output Coupling of Dual-Color Lasers

FRIDAY

Keynote/Invited Talks

Saturday, 21 October A.M   Hunan Room III

Chaired by Hui Jing

09:00 to 09:25
> **Yuxi Liu** (Tsinghua University, Beijing, China)
> Absorption of microwave in driven superconducting artificial atoms

09:25 to 09:50
> **Shan-gui Zhou** (Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, China)
> Superheavy nuclei and new elements

09:50 to 10:15
> **Mingbo Zhou** (Hunan Normal University, Changsha, China)
> Synthesis of N-Containing Heterocycles by Rh/Ag-Catalyzed Cycloaddition Reaction

10:15 to 10:40
> **Xingqiu Chen** (Institute of Metal Research, Chinese Academy of Sciences, Beijing, China)
> Topological Dirac nodal lines in pure metal beryllium and its potential applications

Chaired by Steven R. Kirk

11:00 to 11:35
> **Paul W. Ayers** (McMaster University, Hamilton, Canada)
> Generalized Hirshfeld Atoms in Molecules

11:35 to 12:00
> **Liliana Mammino** (University of Venda, Venda, South Africa)
> Complexes of Hyper-guinones A and B with a Cu^{2+} Ion. A DFT Study

12:00 to 12:25
> **Zheng Xiao** (University of Science and Technology of China, Beijing, China)
> Controlling the quantum states in adsorbed molecular magnets: First-principles based studies

SATURDAY

Keynote/Invited Talks

Saturday, 21 October P.M   Hunan Room III

Chaired by Paul W. Ayers

14:00 to 14:35
> **Frank E. Harris** (University of Utah, Salt Lake City, USA)
> Analytical Computation of Four-Electron Integrals for Extended Hylleraas-CI Wave Functions

14:35 to 15:00
> **Anna Okopińska** (Jan Kochanowski University, Kielce, Poland)
> Entanglement characteristics of bound and resonant few-body states

Chaired by Liliana Mammino

15:45 to 16:20
> **Akitomo Tachibana** (Kyoto University, Kyoto, Japan)
> Quantum Mechanics 100 Years of Mystery is Solved

16:20 to 16:45
> **Jun He** (Central South University, Changsha, China)
> Ultraviolet Nonlinear Optical effects in Black Phosphorus Quantum Dots

SATURDAY

Closing Ceremony

Saturday, 21 October P.M   Hunan Room III

17:00 to 18:00
See you at QSCP-XXIII!

Changsha, China - October 16-21, 2017
http://www.qscp2017.org

Poster Session

Friday, 20 October   19:00 – Corridor outside of Hunan Room III

P-001

>**Taewon D. Kim** (McMaster University, Hamilton, Canada)
>Constructing Arbitrary Multideterminant Wavefunctions

P-002

>**Xiaotian Yang** (McMaster University, Hamilton, Canada)
>Transition State Search and Geometry Optimization

P-003

>**Yilin Zhao** (McMaster University, Hamilton, Canada)
>A tree tensor method for the simultaneous determination of multiple eigenstates

P-004

>**Fanwang Meng** (McMaster University, Hamilton, Canada)
>Procrustes, A Python Package for Matrix Similarity Computation

P-005

>**Tianlong Jiang** (University of Sophia, Tokyo, Japan)
>Research on the Isotopic Effect of the Carboxylation by RuBisCO Using Free Energy Analysis

P-006

>**Wangbin Yu** (Hunan Normal University, Changsha, China)
>Geometry-dependent band shift and dielectric modification of nano-porous

P-007

>**Yanjun Liu** (Hunan Normal University, Changsha, China)
>Complementarity via error-free measurement in a two-path interferometer

P-008

>**Ziran Liu** (Hunan Normal University, Changsha, China)
>First-principles calculations of strength and ductility of magnesium by solid solutes

P-009

>**Yipeng Zhao** (Hunan Normal University, Changsha, China)
>Size-Tunable Band Alignment and Photovoltaic Conversion of MoS2/WSe2 van der Waals Hetero-structures

P-010

>**Mingzhi Wang** (Hunan Normal University, Changsha, China)
>Shadow casted by a Konoplya-Zhidenko rotating non-Kerr black hole

POSTERS

P-011

    Min Yu (Hunan Normal University, Changsha, China)
    Steady and optimal entropy squeezing of a two-level atom with
    quantum-jump-based feedback and classical driving in a dissipative cavity

P-012

    Liemao Cao (Hunan Normal University, Changsha, China)
    The spin-charge transport properties for a graphene-based molecular
    Junction: A first-principles study

P-013

    Chao Kong (Hunan Normal University, Changsha, China)
    Controlling chaotic spin-motion entanglement of ultra-cold atoms via
    spin-orbit coupling

P-014

    Kailei Wang (Hunan Normal University, Changsha, China)
    Understanding the newly observed Ω c states through their decays

P-015

    Chang Liu (Hunan Normal University, Changsha, China)
    Large-scale Synthesis and X-ray Quantitative Analysis of Size-controllable
    Potassium Tungsten Bronze Nanowires

P-016

    Liang Zhang (Hunan Normal University, Changsha, China)
    Interface effect on thermal boundary resistance and phonon thermal
    conductivity in Si/Ge core-shell nanowires

P-017

    Wangjun Lu (Hunan Normal University, Changsha, China)
    Impurity-induced Dicke quantum phase transition and quantum speed-up in
    a cavity-Bose-Einstein condensate system

P-018

    Zhe Zhang (Hunan Normal University, Changsha, China)
    Ab initio Calculations for the Strain Modulation of Electronic Properties of
    Monolayer Black Phosphorus

P-019

    Xiaojun Bao (Hunan Normal University, Changsha, China)
    Systematic study of the mechanism of super-heavy nuclei synthesis

P-020

    Lingling Wang (Hunan Normal University, Changsha, China)
    Insights into the all-metal $[Sb_3Au_3Sb_3]^{3-}$ sandwich complex from a QTAIM
    and stress tensor analysis

POSTERS

P-021

Lingling Wang (Hunan Normal University, Changsha, China)
QTAIM and Stress Tensor Characterization of Intramolecular Interactions
Along Dynamics Trajectories of a Light-Driven Rotary Molecular Motor

P-022

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

P-023

Ping Yang (Hunan Normal University, Changsha, China)
Isomerization of the RPSB chromophore in the gas phase along the torsional
pathways using QTAIM

P-024

Ping Yang (Hunan Normal University, Changsha, China)
Fatigue and Photochromism S_1 Excited State Reactivity of Diarylethenes
from QTAIM and the Stress Tensor

P-025

Tianlv Xu (Hunan Normal University, Changsha, China)
The normal modes of vibration of benzene from the trajectories of stress
tensor eigenvector projection space

P-026

Tianlv Xu (Hunan Normal University, Changsha, China)
A QTAIM and Stress tensor investigation of stereochemistry

P-027

Alireza Azizi (Hunan Normal University, Changsha, China)
Distinguishing and quantifying the torquoselectivity in competitive
ring-opening reactions using the stress tensor and QTAIM

P-028

Yong Liu (Hunan Normal University, Changsha, China)
Polymorph-Selective Assembly and Charge-Transfer Emissions of Organic
Cocrystal Microstructures for Photonic Applications

P-029

Weichang Zhou (Hunan Normal University, Changsha, China)
Synthesis and characterization of topological crystalline
insulators-semiconductor SnTe-ZnTe 1D core-shell hetero-nanostructures

Abstracts of the Talks

Reaction rate-thermodynamic relations and application to single molecule experiments on a biomolecular motor, F_1-ATPase

Rudolph A. Marcus and Sandor Volkan-Kacso

Reaction rate expressions were developed many years ago for "weak overlap" electron transfer reactions, relating the rate of reaction to the thermodynamic driving force (standard free energy of reaction) and to other intrinsic (reorganization energy) properties. Subsequently we extended these ideas to other transfer processes involving a strong interaction of the reactants, such as atom or group transfer from one reactant to another, initially using a "bond energy-bond order "model. The final relationships were subsequently tested by experiments and by detailed quantum mechanical computations, and some examples will be given. More recently in a series of papers (PNAS 2015, 2016, 2017, Quart Rev Biophys, in press) we have extended these ideas to biological motors, focusing initially on F_1-ATPase, where now in the theory one combines physical and chemical processes with a mechanical form of energy, an elasticity of the system. The processes here are the entrance of an ATP (adenosine triphosphate) into a binding pocket of the ATPase, the subsequent ATP hydrolysis and the release of ADP and inorganic phosphate. In the entrance of the ATP into the binding pocket one set of hydrogen bonds is being broken while a new set is simultaneously being formed, so one has a type of "bond breaking-bond forming reaction" and we a similar kinetic-thermodynamic relation that we used earlier for the other transfers. In the analysis we combine this chemistry-based theory with the mechanical energy associated with the motor, by including the latter in the relevant free energy expression. In this way reaction rates were obtained that permitted one to relate different kinds of single molecule experiments (stalling, controlled rotation, and free rotation) to each other and to bulk (ensemble) data. With the theory predictions are made that are compared with experimental rates, with no adjustable parameters.

Interplay between theory & experiment towards novel optics/electronics/spintronics and efficient energy conversion

Kwang S. Kim

The success of novel molecular/material design depends on a comprehensive understanding of inherent atomic/molecular properties, interatomic/molecular interactions, dynamic/transport properties, and collective phenomena. Here I elaborate on the interplay between theory and experiment to design superfunctional nanomaterials and nanodevices. These include intriguing organic nanostructures, large-scale graphene, and functionalized hybrid materials for energy harvesting, fuel cells, gas storage, water remediation, and medical treatment. I will begin with the conceptual understanding of confinement effects in nanomaterials as well as structural changes and phase transitions of 2D materials. The 2D physical and chemical nature of graphene is discussed and the defects, edges, and substrate effects are considered. Assembling phenomena of nanostructures and utilization of the resulting features as devices are addressed. Selective capture of fullerenes and fluorescence-sensing of RNA over DNA are achieved with π+-π, π-π interactions and charged hydrogen bonding. The temperature-driven transient molecular gating in covalent organic molecular frames can store gaseous molecules in ordered arrays. In addition to molecular motion, electronic excitation motions in attosecond timescale are investigated. Using self-assembled nano-scale lenses, hyper-resolution phenomena showing near-field focusing and magnification beyond the diffraction limit are manifested as novel nano-optics. Pt nanoclusters and nanodendrites in a DNA/reduced-graphene-oxide are developed to show outstanding electrochemical catalytic activities. Electron-hole pairing is discussed in perovskite solar cells. Magnetite nanoparticles-graphene hybrid materials showing superparamagnetism are exploited for water remediation. Two-photon assisted N-doped graphene accelerates bone regeneration, and graphene on Cu shows photoluminescence despite of the metallic nature of graphene. Electron/spin transport in molecular electronic/spintronic devices and super-magnetoresistance of graphene nanoribbon spin valves are discussed using non-equilibrium Green function theory plugged in density functional theory. By utilizing Fano-resonance driven 2D molecular electronics spectroscopy using graphene nanoribbon, the hyper-sensitive quantum conductance spectra of a graphene nanoribbon placed across a fluidic nanochannel can lead to fast DNA sequencing including cancerous methylated nucleobases detection. Finally, collective properties of liquids and solids are discussed based on *ab initio* many body molecular dynamics simulations. Phase transitions of materials and the limits of superheating and supercooling of vapor are studied with Monte Carlo simulations using microscopic models with configurational enthalpy as the order parameter.

Electronic processes in C^{q+}-He, H collisions of relevance for fusion plasmas

Alain Dubois

Electron capture processes for carbon ions colliding with atoms or molecules have attracted much attention in the last decades because of their importance in astrophysics and in the treatment of thermonuclear fusion plasmas. In tokamak plasmas, carbon ions are dominant impurities when carbon is used in divertor target plate tiles while helium is abundant as a product in the fusion reaction, and both of them appear at various impact energies and ionization states in the plasma. Therefore, comprehensive and quantitative knowledge of electron capture processes between multiply-charged carbon ions and helium are important for the simulation and diagnostic of fusion plasmas.
In the conference we shall present a theoretical treatment to describe these collisions in a wide impact energy domain where the scattering systems should be treated in non-perturbative approaches. We shall shall present cross sections stemming from our simulation codes concerning collisions involving carbon ion and light neutral elements.

Fully quantum nonadiabatic dynamics in the adiabatic representation

Artur F. Izmaylov

On-the-fly quantum nonadiabatic dynamics for large systems greatly benefits from the adiabatic representation readily available from electronic structure programs. However, conical intersections frequently occurring in this representation introduce nontrivial geometric or Berry phases which require a special treatment for adequate modeling of the nuclear dynamics. I analyze two approaches for nonadiabatic dynamics using the time-dependent variational principle and the adiabatic representation. The first approach employs adiabatic electronic functions with global parametric dependence on the nuclear coordinates. The second approach uses adiabatic electronic functions obtained only at the centers of moving localized nuclear basis functions (e.g., frozen-width Gaussians). Unless a gauge transformation is used to enforce single-valued boundary conditions, the first approach fails to capture the geometric phase. In contrast, the second approach accounts for the geometric phase naturally because of the absence of the global nuclear coordinate dependence in the electronic functions.

Communication Simpliciter: Darwinian Evolution Reconsidered

Erkki J. Brändas

Communication Simpliciter is a stochastic communication hypothesis derived from a quantum mechanical formulation of ensemble representable density matrices. It promotes the emergence of quantum-thermal correlations, based on long-range off-diagonal order with precise thermal conditions fulfilled at specific temperatures. The obtained result, the Correlated Dissipative Ensemble, CDE, is subjected to the Poisson distribution, providing communication channels for cellular recognition, including a proliferated knowledge of neuron correlates. This abstract is entrenched in a *modus operandi* of Darwinian Evolution, which has a philosophical bearing rooted in a self-referential vernacular. The scientific approach is appraised and extended with significant inferences regarding complex enough processes governed by an evolved program. It is finally demonstrated that such an all-inclusive portrait of Nature widens the notion of evolution from the micro- to the cosmic rank of our Universe.

Observe spin-orbit coupling and topological physics for ultracold atoms

Xiongjun Liu

The spin-orbit (SO) interaction plays essential roles in many prominent quantum effects, with which the important topics including spintronics, topological insulators, and topological superconductors emerge in the past over decade. On the other hand, cold atoms with laser-induced SO interactions provide intriguing platforms to explore novel quantum physics beyond natural conditions of solids. In this talk I will present our recent progresses in theory and experiment of observing SO coupling and novel topological physics for ultracold atoms. First, I introduce a hierarchy set of minimal optical Raman lattice schemes for realizing various types of SO couplings and topological phases. The new schemes highlight the high experimental feasibility with long lifetime. Furthermore, I discuss the topological equilibrium and non-equilibrium phases obtained for the optical Raman lattices. Finally, the future important issues in theory and experiment will also be introduced.

Band Gap and Interface Engineering of Low Dimensional Semiconductor Heterostructures

Anlian Pan

Band gaps are one of the most important parameters of semiconductor materials for their optoelectronic applications since they determine the spectral features of absorptions and emission processes. Due to the limited band gaps of natural semiconductors, alloying and heterostructured semiconductors with different band gaps have long been the standard methods of achieving semiconductor structures with new band gaps and functions. In this talk, I will report our recent progress on the band gap engineering of 1D semiconductor nanowires and 2D atomically thin layered materials through controlled vapor growth. Using some examples, I will show how to realize composition graded and interface sharped low dimensional semiconductor heterostructures through composition controlled band gap modulation. The achieved band gap engineered nanostructures can give continuously tuned or white light emission, and can be used to realize multi-color nanolasers, wavelength splitter, asymmetric waveguiding and high-performance photodetectors etc.

Recent Advances in Thermally-Assisted-Occupation Density Functional Theory (TAO-DFT)

Jeng-Da Chai

I will describe the formulation of our recently proposed thermally-assisted-occupation density functional theory (TAO-DFT), the density functional approximations to TAO-DFT (TAO-DFAs), and the hybrid TAO-DFT schemes (i.e., the inclusion of exact exchange in TAO-DFT). In contrast to Kohn-Sham density functional theory (KS-DFT), TAO-DFT is a density functional theory with fractional orbital occupations given by the Fermi-Dirac distribution (controlled by a fictitious temperature), for the study of large ground-state systems with strong static correlation effects. However, existing exchange-correlation energy functionals in KS-DFT may also be adopted in TAO-DFT. Besides, TAO-DFT has similar computational cost as KS-DFT for single-point energy and analytical nuclear gradient calculations, and reduces to KS-DFT in the absence of strong static correlation effects. Relative to our previous TAO-DFAs, the hybrid TAO-DFT schemes are shown to be superior in performance for a broad range of applications, such as thermochemistry, kinetics, and reaction energies.

Halide Perovskite Solar Cell Semiconductors: A Perspective on Their Bonding Scenarios

Pradeep R. Varadwaj,[a,b] Arpita Varadwaj,[a,b] and Koichi Yamashita[a,b]

One of the main interests of energy research is to discover novel photonic devices to resolve the future need for energy. To this end, many varieties of solar cells are discovered with power conversion efficiencies (PCEs) in the $1-30\%$ range, which took decades to accomplish. Trihalide perovskite solar cells with formula BMY_3 are man-made high performance semiconductors with NREL certified PCE of 22.1%, where B is the organic/inorganic cation ($CH_3NH_3^+$ and Cs^+, *etc.*), M is the metal ion (Pb^{2+} and Sn^{2+}, *etc.*), and Y is the halogen derivative (Y = X (X = Cl, Br, I) and/or mixed derivative). This presentation will focus discussions on the fundamental chemical bonding aspects of these and analogous perovskite materials exploited using density functional and coupled cluster theories, NBO, QTAIM and RDG-NCI methods. In specific, the discussion will be centered on the electronic structures, electron density and charge transfer properties of the aforesaid systems in some detail, as well as on the descriptors of bonding interactions that can be transferrable to any other systems for similar studies. The importance of noncovalent interaction in the design of energy materials will be outlined.
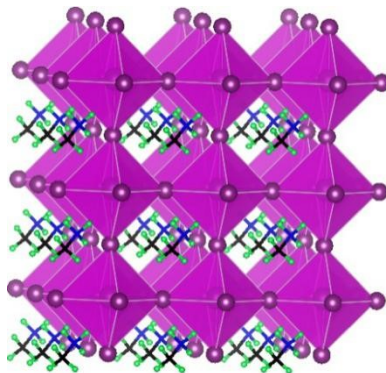
Theoretical study on Criegee intermediate decay processes

Kaito Takahashi

Due to its fast reaction rate with SO_2, carbonyl oxides or Criegee intermediates (CIs) are thought to be important oxidizing agents in the atmosphere. However, in highly humid atmospheric conditions, CIs with hydrogen in the *syn*-conformation of the OO bond, such as CH_2OO, react quickly with water vapor to form hydroperoxy alcohols. Since these alcohols do not react with SO_2, this reaction of CI with water decreases the ability for CIs to act as oxidizing agents in the atmosphere. Furthermore, it has been found that for CIs with an alkyl group in the *syn*-conformation of the OO bond, such as $(CH_3)_2COO$, the hydrogen abstraction unimolecular reaction forming vinyl peroxide can occur at very fast rates. Once again these vinyl peroxides also show low reactivity toward SO_2. Furthermore, CIs have strong absorption in the 300 to 400 nm region, therefore it may absorb solar photons and dissociate the OO bond. Once again the photodissociation product will have small reactivity with SO_2. Therefore, detailed studies on the aforementioned decay processes are required to properly model the CI concentration in atmospheric conditions.

Compared to the detailed studies performed for CH_2OO, CH_3CHOO, and $(CH_3)_2COO$, studies toward CH_3CH_2CHOO is much scarce. In this study, we examine the substituent dependence in the CI's reactivity toward water vapor and unimolecular reaction. Starting from the simplest CI: CH_2OO, we calculated for CH_3CHOO, CH_3CH_2CHOO, and $(CH_3)_2COO$. Furthermore, to clarify the effect of unsaturated carbon bonds, we have also calculated $CH_2CHCHOO$ as well as $CHCCHOO$. Since the CIs that are obtained from the ozonolysis of biogenetic alkenes include unsaturated carbon bonds, we think the systematic study on these C3 CI will provide a good estimate for the CIs in the atmosphere. Furthermore, when one wants to model the photodissociation process, it is important to obtain absolute absorption cross sections for the UV absorption. Utilizing coupled cluster and multireference configuration interaction methods, with quantum simulations, we obtained reaction rate coefficients and UV spectra with high accuracy.

An Enhanced Sampling Method for Searching Conformational Changes of Proteins and Supramolecules

Yasuteru Shigeta

In the computational chemistry and biology, molecular dynamics (MD) simulations with accurate potential energies can trace structural transition to form an ordered-structure from disordered one as found in time series of atomic-level trajectories. However, it might be still difficult to reproduce it because of a time scale issue on MD, i.e. the characteristic time scales of the ordering processes exceed the accessible time scales of conventional MD simulations. To avoid the time scale problem, we have developed an efficient conformational search method, where multiple short-time MD simulations are restarted from selected initial structures taken from previous trajectories with renewed initial velocity. Our algorithms succeeded in finding protein folding pathways for small fast-fording proteins. In this talk the basic algorithms are explained and numerical applications to proteins and supramolecules are shown.

Hawking Radiation for a Proca Field

Mengjie Wang

Hawking radiation is one of the most important phenomena in black hole physics by considering quantum effects near the event horizon. We report our recent work on computing Hawking radiation of a neutral Proca field in a D-dimensional Schwarzschild black hole. Since the mass term introduces a coupling between two physical degrees of freedom of the field, we construct a numerical strategy to solve the coupled system of ordinary differential equations numerically without decoupling. We show how to define the transmission factor for the coupled system from an S matrix and compute them for various modes, masses, and spacetime dimensions. Then we generalize our method to a charged Proca field on the brane for scenarios where the vector bosons are confined within a thin brane. We shall show the charge effect on the transmission factor as well as the corresponding Hawing radiation. Finally, we analyze the bulk/brane emission rate.

Time-dependent wavepacket diffusive method and its applications to carrier quantum dynamics in organic materials

Yi Zhao

The carriers in organic materials commonly follow hopping-type motions because of strong carrier-phonon interactions. However, they can also present a band-like behavior in well-performed organic crystals or mixed inorganic-organic materials. Therefore, the carrier quantum dynamics should be described by a unified way covering from band-like to hopping-type motions. Such a unified method for large systems still meets a great challenge in theoretical chemistry. Focusing on this problem, we have proposed a time-dependent wavepacket diffusion method (TDWPD). In the methods, the effects of carrier-phonon interaction and inter- or intra-molecular electronic couplings are considered as the fluctuations on carrier dynamics. It has been demonstrated that the TDWPD computational cost is similar to that of mixed quantum-classical methods for complex systems, but it overcomes their deficiency that the detailed balance principle is broken down, also includes nuclear tunneling effect and correctly predicts a long-time dynamics behavior. We further present how to combine electronic structure calculations and molecular dynamics simulations with the TDWPD to reveal the carrier dynamics in realistic organic semiconductors, such as exciton energy relaxation and dissociation, mobility of electron and hole and singlet fission.

New Implementation of Static-Dynamic-Static second order perturbation theory (SDSPT2)

Yibo Lei[a], Wenjian Liu[b], Mark R. Hoffmann[c]

A new Static-Dynamic-Static second order perturbation theory (SDSPT2) based multi-reference Correlation computations have been implemented with the involvements of Graphical Unitary Group Approach (GUGA) and Dyall Hamiltonian to improve the original SDS strong correlation calculation. The implementation has employed hole-particle correspondence and internal contraction of the whole Q space to reduce the computational complexity. Particularly, the dimension of Q space relies only on the orbitals but not the reference configuration states (CSFs). Additionally, the involvement of Dyall Hamiltonian can maintain more dynamic correlations between CSFs in the Q subspaces and further separate the reference space (P) and perturbation space (Q) in comparison with the original SDS-MS-MRPT2. Eventually, the new SDS-MS-MPRT2 has the following characteristics: 1) The flexibility between P and Q space as superior as the original one; 2) The large systems with transitional metals can be calculated with the reduction of complexity by new computational strategies; 3) Avoid the existence of intrude state issue with the improvement by Dyall Hamiltonian; 4) More dynamic correlations have been contained particularly on the dissociation region.

Model Wavefunctions for Strongly-correlated systems

Paul A. Johnson

Established methods of quantum chemistry are based on the orbital picture: electrons occupy orbitals and interact with the average field of the other electrons. The wavefunction is a Slater determinant of the occupied orbitals. This picture is convenient when it's possible to unambiguously label orbitals as occupied or unoccupied. Systems of this type are weakly-correlated and generally well-described by existing methods. When it's difficult to classify orbitals as occupied or unoccupied, the wavefunction cannot be described by a Slater determinant, and the number of important Slater determinants grows exponentially with the system size. Systems of this type are strongly-correlated. The goal of our work is to develop affordable variational techniques for strongly-correlated systems. Our approach uses wavefunctions from integrable models, which will serve as starting points for perturbation theories. This approach will be outlined with the eigenvectors of Richardson-Gaudin models.

On the mutagenicity of 5-bromouracil: Is tautomerism to blame?

Tanja van Mourik

The mutagenicity of unnatural DNA base analogues is among their most salient properties, but its mechanism is a long-running controversy. The "rare tautomer hypothesis", in which analogues disrupt standard purine/pyrimidine base-pairing by forming tautomers that are vanishingly unfavorable for natural bases, is virtually received wisdom among biologists. However, its physical basis has been called into doubt by chemists, who question the thermodynamic stability of minor base tautomers. 5-Bromouracil (5BrU) is an archetypal analogue mutagen: the simple replacement of the methyl group of thymine with bromine dramatically increases the mutagenic rate following incorporation into DNA. Using DFT calculations on 5BrU in nanodroplets we have shown that explicit waters considerably increase the stability of the enol tautomer, relative to that of uracil. These calculations however do not give information on the dynamics of the proton transfer. Using constrained Car–Parrinello molecular dynamics calculations, we show that the bulk-water-assisted deprotonation of BrU at N3, followed by reprotonation at the "mutagenic" O4 site, is indeed more favorable for BrU than for uracil at 320 K.

Synthetic Chemistry of Porphyrin Arrays and Porphyrinoids

Jianxin Song

Highly conjugated multi-porphyrin arrays have received much attention in light of their potential applications in optoelectronic devices, sensors, photovoltaic devices, non-linear optical (NLO) materials, photodynamic therapy (PDT) pigments, and light-harvesting models. Linear, cyclic,star shaped porphyrin arrays have been extensively explored as synthetic models of photosynthetic antenna and functional hosts possing convergent multi-dentate coordination sites. The manipulation of interporphyrinic interaction is often essential to achieve desirable electronic and photophysical properties. Palladium catalyzed cross coupling of borylated porphyrins and aryl halides, it is widely used to synthesize some porphyrin arrays which could not be obtained in other strategies. In this topic, we will introduce some interesting work from our laboratories.
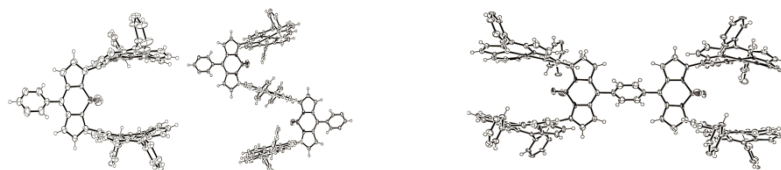
Novel Magnetoelectric Multiferroicity in A-site Ordered Cubic Perovskite Oxides

Youwen Long

In magnetoelectric multiferroic (FM) materials, long-range spin ordering and ferroelectric polarization coexist and even strongly couple with each other. As a result, one may realize magnetic control of electric polarization as well as electric control of magnetism, providing a promising multifunctional material for next-generation advanced spintronic devices. Perovskite is one of the most important FM materials. Magnetoelectric multiferroicity is not expected to occur in a cubic perovskite system due to the high structural symmetry. By versatile measurements in magnetization, dielectric constant, electric polarization, neutron and x-ray diffraction, as well as theoretical calculations, we reveal that the A-site ordered perovskite oxide $LaMn_3Cr_4O_{12}$ with cubic symmetry is a novel spin-driven MF system with strong magnetoelectric coupling effects. When a magnetic field is applied in parallel (perpendicular) to an electric field, the ferroelectric polarization can be enhanced (suppressed) significantly. The unique MF phenomenon observed in this cubic perovskite cannot be understood by conventional spin driven microscopic mechanisms. Instead, a nontrivial effect involving the interactions between the A-site Mn^{3+} and B-site Cr^{3+} magnetic sublattices plays a crucial role. In addition, in another A-site ordered perovskite oxide $BiMn_3Cr_4O_{12}$, we for the first time realize both large ferroelectric polarization and strong magnetoelectric coupling.

Constraint Structure Optimization for Minimum Energy Intersystem Crossing Point

Jun-ya Hasegawa

Metal complexes show various functionalities related to intersystem crossing (ISC). Dioxygen binding to haemoglobin would be one of the most common examples. Since after Pauling's finding, it is well known that the O_2 molecule in the triplet ground state is bound at quintet deoxyheme and becomes oxyheme in singlet ground state. Apparently, this process involves intersystem crossing at a certain point of the reaction pathway. Such spin-state changing reactions are sometimes understood and recognized as two-state reactivity concept. In these reactions, the ISC point becomes a transition state. Therefore, finding the ISC structure, particularly minimum energy point on the ISC seam, is important to understand the catalytic reactivity of the complex. In this presentation, we summarize our recent studies on spin-state crossing from transition metal chemistry to biological triplet quenching, such as O_2 binding to hemoglobin, spin-block phenomena in molybenocene, and triplet quenching at cartenoid.

Towards the inclusion of dissipation in quantum time dependent mean field theories

Eric Suraud , Congzhang Gao

Mean field provides an essential starting point to understand the dynamics of numerous many-body systems ranging from nuclei to molecules, clusters and nano structures. Beyond structural or low energy properties, the analysis of dynamical processes, especially beyond the linear response domain requires the account of correlations beyond mean field, especially incoherent ones. We discuss in the present work some extensive studies we have led to include incoherent correlations on top of Time Dependent LDA or Time Dependent Harthree Fock (TDHF) approaches which represent archetypical mean fields approaches in the time domain. We propose a quantum Relaxation Time Ansatz (RTA) providing an approximate quantum kinetic treatment and a stochastic extension of mean field, known as Stochastic TDHF. The RTA has allow us too access realistic laser irradiation scenarios and study in particular the impact of dissipation on electron emission in moderate size clusters. The STDHF (or Stochastic TDLDA) approach is much richer but still at a more schematic level. We have nevertheless explored it in simple molecular systems and been able to analyse its capabilities in detail. Finally we have been able to develop a simplified approach coined Average STDHF (ASTDHF), which allows to treat large systems even at moderate excitations, which opens the door to the study of realistic 3D systems.

Quinone based building blocks for molecular electronics

Herbert A. Früchtl

It has been shown that azophenine (1,4-diamino-3,6-diimino-1,4-cyclo-hexadiene) adsorbed on a Cu-(110) surface displays controlled switching behavior between tautomeric conformations when exposed to a current through an STM tip. Thus it could be used as a molecule-sized memory element.The prerequisites of such behavior are:
- Two states of similar energy, separated by a not too high barrier.
- Different electronic behavior, such as conductivity, between the two states.

If such behavior could be reproduced away from the surface, similar molecules, based on a quinone-like core, could be used as switches or transistors for molecular electronics. We will present initial results for tautomerisation barriers and electron transport properties of candidate molecules between electrodes to assess their suitability as components in more complex molecular electronic networks.

Elucidation of the Structure and Properties of Surface Species on Ceria Catalysts by Quantum Chemical Modeling

Georgi N. Vayssilov, Hristiyan A. Aleksandrov, Petko St. Petkov, Iskra Z. Koleva.

Using quantum chemical modeling with periodic boundary conditions we investigated interaction of platinum clusters and isolated ions with cerium dioxide support, as well as the stability and vibrational frequencies of different surface species formed upon adsorption of gas molecules – CO, CO_2, NO, H_2O, etc. Ceria was modeled as regular slab of $CeO_2(111)$ surface and as ceria nanoparticle and the computational results were compared with data from relevant experimental methods. For Pt/CeO2 system we were able to explain the strong dependence of the catalytic activity on the morphology of the support by oxygen spillover onto the platinum particle. The electronic state of the different types of platinum species deposited on ceria was characterized by CO adsorption. CO was also found to assist decomposition of platinum clusters supported on nanostructured ceria into cationic platinum dicarbonyls. Our simulations allowed re-assignment of the experimentally observed infrared bands to specific structures of surface carbonates, hydrogen carbonates and formates on ceria. Based on computational results and the evolution of the infrared spectra we established for the first time two new types of surface intermediates on reduced ceria – azides, N_3^-, and nitric oxide dianions, NO^{2-}. We are grateful for the support from the H2020 project Materials Networking.

Theoretical chemistry for space chemistry

Dahbia Talbi

Almost 200 molecules have been detected so far in the interstellar medium and circumstellar shells among which 60 are organic compounds with more than 6 atoms with a straight-chain backbone. Understanding the formation and destruction paths of these molecules both in the gas-phase and in/on solids (cosmic grains, ices) is crucial to diagnose the physical condition of the environments where this chemistry take place. There is therefore a strong demand from the astrophysical community for its study and theoretical chemistry had become an important tool for such a task specially when experiments are not possible because of the unstable species involved (radicals, ions) or because of the extreme conditions of temperatures (10-100K) and densities (10^2-10^8 particles/cm^3) to be considered and not always reproducible in the laboratory. To illustrate the role of theoretical chemistry in understanding space chemistry I will present few theoretical studies that have elucidated astrochemical problems.

A fifth rung density functional that correctly describes both density and energy

Xin Xu

Computational methods based on density functional theory (DFT) are the most widely used tools in physics, chemistry, and materials science, while finding the reliable density functional approximations (DFAs) to the exact functional is a central task in theoretical physics and chemistry. Recently, Medvedev et al. (Science, 355 (2017) 49) argued that DFA development is "straying from the path toward the exact functional". The exact functional should yield both exact energy and density for a system, nevertheless, they found that many newly developed DFAs failed to improve both simultaneously. The 128 functionals examined by Medvedev et al. include only the first four rungs of "Jacob's Ladder" of Perdew. Here, we show that the XYG3 type of doubly hybrid functionals, a functional on the top fifth rung, can well describe both density and energy, demonstrating one feasible way to approach the exact functional.

Synthesis and Reactivity of Lutetacyclopentadiene

Ling Xu, Junnian Wei, Yuchen Wang, Yang Wang, Zitao Wang, Wenxiong Zhang* and Zhenfeng Xi

The first well-defined lutetacyclopentadienes are synthesized from pentamethylcyclopentadienyl lithium (Cp*Li), 1,4-dilithio-1,3-butadienes, and $LuCl_3$. The lutetacyclopentadiene shows excellent reactivity towards some small molecules, such as pivalaldehyde, element Se, carbon dioxide, and isonitrile to efficiently construct 3-, 5-, 7-, 8-, and 9-membered rare-earth metallacycles. Both monoinsertion and double-insertion of two Lu-Csp^2 bonds are observed. Specially, the reaction between lutetacyclopentadiene and isonitrile affords [3,5,5]-fused metallacycles. Furthermore the reactivity of lutetacyclopentadiene towards N,N'- diphenylcarbodiimide (DPC) is systematically investigated to efficiently construct three types of new N-containing fused cyclic complexes. The outcome of these reactions significantly depends on the metal center, the concentration of LiCl, the number of equivalents of DPC, and the solvent. By using DFT calculations we understand the reaction in depth and the results of DFT calculations agree well with the experimental results that the coordination of LiCl plays an important role in the branch of the reaction routes.

Ensemble Density Functional Theory Method for Modeling Dynamics of Excited States

Michael Filatov

Ensemble density functional theory (eDFT) is a novel theoretical formalism capable of exact description of strong non-dynamic electron correlation effects in the ground and excited states of electronic systems. eDFT provides a rigorous framework for time-independent approach to the calculation of excited states. Practical implementation of eDFT in the form of spin-restricted ensemble-referenced Kohn-Sham (REKS) method and its state-averaged (SA-REKS) and state-interaction (SI-SA-REKS or SSR) extensions enable one to describe correctly the shape of the ground and excited potential energy surfaces of molecules undergoing bond breaking/bond formation reactions including features such as avoided crossings and conical intersections crucial for theoretical modeling of non-adiabatic processes. In my talk, I will review the basic principles behind the REKS methodology and aspects of its implementation. Computation of the analytic energy gradient and the non-adiabatic coupling vectors between the ground and excited states will be presented along with several examples of investigation of the non-adiabatic dynamics of excited states in retinal chromophore and its simplified models. Implementation of the REKS methodology for the calculation of multi-excitonic states will be described and application of the new methodology to modeling of multi-chromophoric systems, including systems involved in the singlet exciton fission, will be presented.

Interaction Entropy for Binding Free Energy

John Z.H. Zhang, Xiao He

The theoretical calculation of host-guest binding free energy is a grand challenge in computational biology. Accurate prediction of critical residues along with their specific and quantitative contributions to protein-protein binding free energy is extremely helpful to reveal binding mechanisms and identify drug-like molecules that alter protein-protein interactions. In this talk we develop an efficient approach to computing quantitative residue-specific contributions to protein-protein binding free energy. The approach provides explicit contribution of the entropic loss in binding free energy of individual residues directly from fluctuation of the interaction energy in MD simulation. Studies for an extensive set of realistic protein-protein interaction systems showed that by including the entropic contribution, the computed residue-specific binding free energies are in better agreement with the corresponding experimental data. Predictions of hot stops for some important protein-protein interactions are discussed.

Theoretical Studies on Terpenoids Biogenesis

Yongheng Wang, Fan Zhang, Jingwei Zhou, Ruibo Wu[*]

One of the bottlenecks in modern drug discovery is the limitation of chemical diversity for drug screening, biosynthesis are effective ways to enhance the scaffold diversity of chemical libraries. For example, Farnesyl Pyrophosphate cyclase (FPPC) could catalyze linear sesquiterpene substrates to generate more than 300 known monocyclic, bicyclic, and tricyclic sesquiterpene products with different carbon skeletons. So far, natural products are the most important sources of new drug discovery. Enzymatic catalysis mechanism, which is the central to understand the biogenesis and diversity of natural products, would shed bright lights on the rational drug design and protein engineering. Herein, I will share some cases studies on illuminating the complex biosynthetic mechanism of several cyclic terpenoinds by employing DFT/MM MD simulations.

A unified theoretical framework for mapping models for the multi-state Hamiltonian and a unified thermostat scheme for quantum/classical statistics

Jian Liu

The presentation is consist of two parts. We first propose a new unified theoretical framework to construct equivalent representations of the multi-state Hamiltonian operator and present several approaches for the mapping onto the Cartesian phase space. After mapping an F-dimensional Hamiltonian onto an $F+1$- dimensional space, creation and annihilation operators are defined such that the $F+1$- dimensional space is complete for any combined excitations. Commutation and anti-commutation relations are then naturally derived, which show that the underlying degrees of freedom are neither bosons nor fermions. This sets the scene for developing equivalent expressions of the Hamiltonian operator in quantum mechanics and their classical/semiclassical counterparts. Six mapping models are presented as examples. The framework also offers a novel way to derive such as the well-known Meyer-Miller model.

We then show a unified second-order scheme for constructing simple, robust and accurate algorithms for typical thermostats for exact quantum/classical statistics for the canonical ensemble. The scheme consistently improves the efficiency for evaluating all quantum thermodynamic properties for any type of thermostat. Even when the Born-Oppenheimer approximation is broken, the unified scheme offers a powerful and accurate tool for studying non-adiabatic systems in thermal equilibrium.

Exotic hadrons near threshold

Qiang Zhao

We show that exotic hadrons beyond the conventional quark model turn out to be easier to identify when near-threshold S-wave strong couplings are present. This phenomenon raises critical questions on the understanding of structures and dynamics for exotic hadrons. Meanwhile, it also implies that special kinematic effects can arise from near-threshold interactions. In particular, we will demonstrate that the so-called "triangle singularity" mechanism can produce unique peaking structures and a better understanding of this mechanism is necessary for a proper interpretation of a lot of newly observed exotic hadron candidates.

Giant Rashba spin splitting in supported stanene

Mingxing Chen

Free stanene, the tin counterpart of graphene, was predicted to be a large-gap quantum spin Hall insulator. Unlike graphene, which can be mechanically exfoliated from graphite, stanene have to be grown on substrates. Recent experiments reveal that the strong hybridization between the grown monolayers and the substrates significantly modify the electronic bands of stanene at K. Based first-principles calculations we propose that Al 2 O 3 is an ideal substrate for the growth of stanene due to the small lattice mismatch between Al 2 O 3 (0001) surface and stanene. We find that the strong interaction with the substrate not only stabilizes the low-buckled two-dimensional structure of stanene, but also gives rise to a large spin-orbit gap at Γ. Moreover, the peculiar substrate-stabilized structure induces a giant Rashba spin splitting in stanene, possessing excellent potential for applications in spintronics.

Center of Mass Momentum Dependent Interaction Between Ultracold Atoms

Peng Zhang

We show that a new type of two-body interaction, which depends on the momentum of the center of mass (CoM) of these two particles, can be realized in ultracold atom gases with a laser-modulated magnetic Feshbach resonance (MFR).

Here the MFR is modulated by two laser beams propagating along different directions, which can induce Raman transition between two-body bound states. The Doppler effect causes the two-atom scattering length to be strongly dependent on the CoM momentum of these two atoms. As a result, the effective two-atom interaction is CoM-momentum dependent, while the one-atom free Hamiltonian is still the simple kinetic energy.

WEDNESDAY

Computer Spectrometers!

Nike Dattani

Ideally, the cataoging of spectroscopic linelists would not demand laborious and expensive experiments. Whatever an experiment might achieve, the same information would be attainable by running a calculation on a computer. Kolos and Wolniewicz were the first to demonstrate that calculations on a computer can outperform even the most sophisticated molecular spectroscopic experiments of the time, when their 1964 calculations of the dissociation energies of H_2 and D_2 were found to be more than 1 cm larger than the best experiments by Gerhard Herzberg, suggesting the experiment violated a strict variational principle. As explained in his Nobel Lecture, it took 5 more years for Herzberg to perform an experiment which caught up to the accuracy of the 1964 calculations.

Today, numerical solutions to the Schrödinger equation, supplemented with relativistic and higher-order quantum electrodynamics (QED) corrections can provide ro-vibrational spectra for molecules that we strongly believe to be correct, even in the absence of experimental data. Why do we believe these calculated spectra are correct if we do not have experiments against which to test them? All evidence seen so far suggests that corrections due to gravity or other forces are not needed for a computer simulated QED spectrum of ro-vibrational energy transitions to be correct at the precision of typical spectrometers. Therefore, a computer-generated spectrum calculated properly can be considered to be as good as one coming from a more conventional spectrometer, and this has been shown to be true not just for the H_2 energies back in 1964, but now also for several other molecules.

So, are we at the stage where we can launch an array of calculations, each with just the atomic number changed in the input file, to reproduce the NIST energy level databases? Not quite. But I will show that for the $6e^-$ molecule Li_2, we have reproduced the vibrational spacings to within 0.001 cm of the experimental spectrum, and I will discuss present-day prospects for replacing laborious experiments for spectra of certain systems within the reach of today's "computer spectrometers".

Macroscopic Quantum Superposition in Cavity Optomechanics

Jieqiao Liao

Quantum superposition in mechanical systems is not only key evidence for macroscopic quantum coherence, but can also be utilized in modern quantum technology. Here we propose an efficient approach for creating macroscopically distinct mechanical superposition states in a two-mode optomechanical system. Photon hopping between the two cavity-modes is modulated sinusoidally. The modulated photon tunneling enables an ultrastrong radiation-pressure force acting on the mechanical resonator, and hence significantly increases the mechanical displacement induced by a single photon. We study systematically the generation of the Yurke-Stoler-like states in the presence of system dissipations. We also discuss the experimental implementation of this scheme.

Defect-induced exceptional point in phonon lasing

Hui Jing

Exceptional points (EPs) are non-Hermitian degeneracies which occur when two or more modes of a physical system coalesce in their resonant frequency and their rate of decay. In systems where the loss of one mode is balanced by the gain in another mode, EPs are generally referred to as parity-time symmetry breaking point. EPs lead to many counter-intuitive phenomena such as lossinduced transparency, invisible sensing, loss-induced optical revival, single-mode lasing, and topological energy transfer. On the other hand, the emerging field of optomechanics has led to many important applications, including the striking observation of a phonon laser, which provides the core technology to integrate coherent phonon sources and devices. However, defects in materials, which have been traditionally considered to be detrimental for achieving phonon lasers, have been neglected in previous works. Here we show that contrary to this traditional view, material defects can lead to the emergence of an EP, beyond which the mechanical gain and the phonon number start to increase significantly with increasing loss. This indicates a novel and counterintuitive way to improve the performance of a phonon laser i.e., by tuning lossy defects, instead of adding any active dopants.
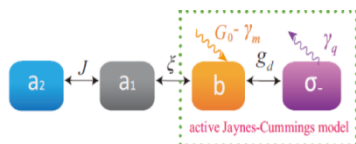

Fig. 1 Defect-induced EP in phonon lasing: the mechanical mode, when operates in lasing regime, forms an effective parity-time system with the two-level-system (TLS) defect

Real time excited state dynamics of alkali-doped helium nanodroplets: A TDDFT study

Maxime Martinez,[1] François Coppens,[1] Manuel Barranco,[1,2,3] Nadine Halberstadt[1] and Martí Pi[2,3]

We report a theoretical investigation of the excited state dynamics of alkali-doped He nanodroplets in real-time. He nanodroplets are intriguing, quantum fluid objects of finite size. Doping them with alkali atoms makes them a particularly interesting model to study the fate of an excited atomic or molecular system in or on them. Alkali atoms are known to sit in a dimple at the droplet surface, and to usually desorb upon electronic excitation, except for Rb and Cs excited close to the gas phase D1 transition. In addition, the alkali atom can bring along one or a few helium atoms and desorb as an exciplex. During the past few years, several real time dynamics experiments have been conducted on superfluid helium nanodroplets doped with alkali atoms using femtosecond pump-probe laser techniques. In particular, the combination of fs pump-probe spectroscopy with velocity map imaging has allowed to clearly disentangle complex formation, desorption, and ion solvation.Helium density functional theory (He-DFT) approach and its time-dependent version (He-TDDFT) are the best compromise between accuracy and feasibility to study the stability and real time dynamics of doped helium droplets with a size comparable to experiments. We have used He-DFT and He-TDDFT to model the photodissociation dynamics of Rb and Cs, for which fs pump-probe spectroscopy combined with velocity map imaging experiments have been conducted. The results of the simulation can therefore be directly compared with experiments. For Rb excited to 5p and 6p, desorption occurs on strikingly different time scales (~100 vs 1 ps, respectively). The comparison between theory and experiment indicates that desorption proceeds impulsively for 6p excitation, whereas it is intermediate between impulsive dissociation and complex desorption for 5p excitation.We have also applied He-DFT and He-TDDFT to study the photodissociation of potassium atoms from helium droplets. The desorption lifetimes obtained experimentally appear to be contradictory. In addition, potassium is very interesting limiting case between classical and quantum behavior. We will show results for K(4p) excitation in an attempt to solve the controversy, and for (5s) excitation in order to explore quantum effects in the desorption.

Chemical Transferability of Functional Groups Follows from the Nearsightedness of Electronic Matter

*Stijn Fias[a,b] *, P. Geerlings [a), and Paul W. Ayers[b)*

The nearsightedness of electronic matter (NEM) is a concept in quantum chemistry with important implications, but it has received relatively little attention and, until now, has never been studied numerically on molecules. The concept of NEM, introduced by Kohn, states that for systems with many electrons at constant electronic chemical potential, there is a radius, R, for every point in space, r_0, such that no change in external potential farther than R units from r_0 will ever cause the electron density at r_0 to change by more than a maximum value $\Delta\rho(r_0,R)$, no matter how large the perturbation. Put differently, the particle density at r_0 cannot "see" any perturbation beyond R with an accuracy beyond $\Delta\rho(r_0,R)$. Kohn and Prodan proved the concept for some model systems, but numerical data on real molecules are, until now, lacking. One feels the importance of this principle, as it must be connected with the issue of transferability of atoms and functional groups from one molecule to another, a rational frequently used in organic chemistry.When looking at Kohn's argument one recognizes $\Delta\rho(r_0)$ and $\Delta v(r')$ suggesting that the linear response function, connects both. However, one of Kohn's assumptions is the condition of constant electronic chemical potential μ (and not of constant number of electrons, N, as in). One thus has to look at $(\delta\rho(r)/\delta v(r'))_\mu$, which is minus the softness kernel, , and is related to the linear response function by the Berkowitz-Parr relation: where is the Fukui function and   the hardness of the system. Using this Berkowitz-Parr relation we are able to calculate the softness kernel in molecules analytically for the first time. We present and discuss the softness kernel for saturated and unsaturated molecules and the results show that is more nearsighted than , proving the transferability of functional groups at constant electronic chemical potential numerically for the first time. This locality principle elucidates the transferability of functional groups in chemistry.

Exploring a new Heisenberg's error-disturbance relation using trapped ultracold ion system

Mang Feng

Heisenberg's uncertainty relations have played an essential role in quantum physics since its very beginning. Here we report experimental tests of one of the new Heisenberg's uncertainty relations using a single ultracold $^{40}Ca^+$ ion trapped in a harmonic potential. By two independent methods, we verified a new uncertainty inequality based on a general error trade-off relation for joint measurements on two compatible observables. The lower bound of the uncertainty, as observed, is satisfied in a state-independent fashion. The work provides a prototypical determination of ultimate joint measurement error bounds with potential applications in quantum information science for high-precision measurement and information security, and will stimulate broad interests in various fields associated with quantum mechanics.

Formulation of QTAIM for 2-Component Relativistic Hamiltonians

James S. M. Anderson

The quantum theory of atoms in molecules (QTAIM) as originally formulated is a successful method for computing atomic properties in a quantum mechanical framework. Prof. R.F.W. Bader and coworkers showed that AIM satisfies the Schwinger principle of stationary action and as such justifying its utility for computing atomic properties in a nonrelativistic setting. Relativity must be accounted for when computing properties of chemical systems that include nuclei with atomic number larger than 37. In this presentation I will demonstrate how to formulate QTAIM to include relativistic effects in defining a proper quantum subsystem that satisfies Schwinger's principle of stationary action for two-component Hamiltonians. This will be carried out in an analogous way to the non-relativistic treatment of QTAIM. I will concentrate on some popular two-component Hamiltonians including the popular scalar-relativistic zeroth-order regular approximation (SR-ZORA).

Unitary Group Adapted Multi-reference Theories: State Universal and State Specific Approaches

Debashis Mukherjee

I will present a succinct account of formulations and implementations of a suite of State Universal (SU) and State Specific (SS) Multi-reference Coupled Cluster (MRCC) theories. These are explicitly unitary group-adapted (UGA) and thus do not suffer from spin-contamination, unlike the commonly used spin-orbital based approaches. We will refer to them as UGA-SUMRCC and UGA-SSMRCC respectively. Time permitting, I will also discuss the perturbative analogue of the SS version which we call UGA-SSMRPT2. The formalisms invoke a new normal ordered multi-exponential type cluster Ansatz analogous to, but different from, the one suggested by Jeziorski and Monkhorst (JM). Unlike in the JM Ansatz, the cluster operators are defined in terms of spin-free generators of the Unitary Group. The excitation operators are non-commuting in general, and this is the reason for invoking the normal ordered multi-exponential Ansatz to simplify the working equations.

The UGA-SUMRCC follows from the Bloch equation involving a suitable active space, while the UGA-SSMRCC theory requires suitable sufficiency conditions to arrive at a well-defined set of equations for the cluster amplitudes. While the more conventional projection equations necessitates that only the linearly independent excitations for a given model function, one can alternately use the amplitude equations by invoking sufficiency conditions for them. A comparative numerical study of the performance of the projection equations and the amplitude equations will be presented. As a sub-set of the UGA-based formalism, it is profitable to look into the relative performance of an open shell UGA version (UGA-OSC) for obtaining the core ionization potential of a closed shell state with one 'heavy' atom, using the spin-free portion of the Dirac operator a la Dyall. Both the spin-free 4-c (SF 4c) and the exact spin-free two component (SFX2c-1e) relativistic hamiltonians have been used in our UGA-OSC theory.

The perturbative approximation to any MRCC presents a unique set of challenges with regard to maintaining the desirable characteristics of the corresponding CC theory and including the essential physics in a compact manner. If time permits, I will discuss UGA-SSMRPT2, a perturbative approximant to the UGA-SSMRCC via amplitude equations, as a prototype and show that it has the potentiality of describing the PES of large systems in a size-extensive, size-consistent and intruder-free manner.

Nonadiabatic *ab initio* Molecular Dynamics with PME-ONIOM Scheme of Photoisomerization Reaction between 1,3-Cyclohexadiene and 1,3,5-*cis*-Hexatriene in Solution Phase

Shinkoh Nanbu

The ultra-fast photoisomerization reactions between1,3-Cyclohexadiene (CHD) and 1,3,5-cis-Hexatriene (HT) in both hexane and ethanol solvents were revealed by nonadiabatic ab initio molecular dynamics with a particle-mesh Ewald (PME) summation method and our Own N-layered Integrated molecular Orbital and molecular Mechanics (ONIOM) model (PME-ONIOM) scheme. Zhu-Nakamura trajectory surface hopping method (ZN-TSH) was employed to treat the ultra-fast nonadiabatic decaying process. The results for hexane and ethanol simulations reasonably agree with available experimental data. The high nonpolar-nonpolar affinity between CHD and the solvent was observed in hexane, which definitely affected the S1 lifetimes, the product branching ratio of CHD:HT (40:60 by S1-excitation), and solute (CHD) dynamics. In ethanol, however, the CHD solute was isomerized in the solvent cage caused by the first solvation shell. The CHD:HT product-ratio was 80:20 by S1, which quite differs from in hexane. The photochemical dynamics also results in the similar property to the process appeared in vacuo (isolated CHD dynamics). Cage would appear because of induced dipole moment of CHD in ethanol; dipole moment in S1 state was found to be 0.85* Debye.

Advantages of Structural Designs in Natural Light-Harvesting Complexes and Advanced Spectroscopic Methods for Tracking Energy Transfer

Hui Dong

Recent applications of ultrafast spectroscopy with sub-picosecond laser enable direct measurements of dynamics of light capture and subsequent energy transfer in light-harvesting processes. Observations of long-lived coherence in these experiments have trigged a new research area to understand the very initial processes of light-harvesting, and their relations to the corresponding photosynthetic structures. In this talk, I will introduce our understanding of the physical origin of long-lived coherence during energy transfer, a new method of tracking energy transfer, and our recent proposed protection mechanism against damage by excess sunlight in the ring antennas of light-harvesting complexes.

THURSDAY

Design of TADF-Utilizing OLEDs

Alia V. Tadjer

In order to attain fine tuning of color and intensity of the light emitted from potential organic light-emitting diodes (OLEDs), molecular design based on a donor-spacer-acceptor model is undertaken. Triplet harvesting is a route to increasing emission efficiency, which can be achieved by thermally activated delayed fluorescence (TADF) when triplet and singlet excited states are quasi degenerate. Using density functional theory, the relevant singlet−singlet and triplet-singlet energy gaps corresponding to absorption or emission transitions of the compounds are computed to simulate the electroluminescent spectrum. Relations between some spectral and structural properties are proposed. Guidelines for systematic improvement of the molecular characteristics are outlined.

**Toward Controlling Complex Chemical Reactions in the Molecular Aggregation States
-From Multiscale Simulation to Computational Molecular Technology-**

Masataka Nagaoka

When we treat computational chemically diffusion processes and chemical reactions in "molecular aggregation states" where a large number of atoms and molecules are gathered in condensation, it is really difficult even with traditional classical molecular simulations to determine the long-term properties and stereochemical characteristics. Under the circumstances, we have recently developed Red Moon methodology, a new efficient and practical 'atomistic' simulation methodology combining Monte Carlo (MC) and molecular dynamics (MD) method with a Rare Event-Driving Mechanism for large-scale chemical reaction systems. In this talk, several applications of Red Moon methodology are shown from the practical viewpoint of molecular controlling of complex chemical reactions, stereochemistry and aggregate structures. First, in investigating the formation process of solid electrolyte interphase (SEI) film in lithium-ion batteries (LIB) and sodium-ion batteries (NIB), it is shown that the SEI film formation is strongly sensitive to the small structural difference of electrolyte molecules and the additive molecules. Second, we take the aromatic polyamide membrane, i.e., FT-30, and show interestingly that the simulations of the ratio 1:4 and 1:1 are in good agreement with the experimental ones by XPS and RBS, respectively. I would like to mention the future applications of the, introducing briefly the latest results until the day of this symposium.

Developments in QTAIM and Stress Tensor Theory

Samantha Jenkins

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

- New interpretation of the Ramachandran plot applicable to peptides and molecular motors.
- The normal modes of vibration of benzene.
- The dynamics of fast and slow trajectories of a light-driven rotary molecular motor.
- Understanding fatigue and photochromism of the S_1 excited state of diarylethenes.
- The functioning of doped azophenine switches.
- Distinguishing and quantifying the torquoselectivity in competitive ring-opening reactions.
- Isomerization of the RPSB chromophore in the gas phase along the torsional pathways using QTAIM.
- Investigation of stereochemistry.
- Demonstrated standard treatments of relativistic effects insufficient for the $[Sb_3Au_3Sb_3]^{3-}$ complex.

Electronic coupling and rates for Singlet Fission

Chao-Ping Hsu

In the simulation of dynamics with curve-crossing, the states involved are close in energy, and the Born-Oppenheimer approximation breaks down. The dynamics is better described with diabatic states, which generally require additional conditions in their definition and description. Even though diabatic states are originally defined as the eigenstates of the kinetic energy operator, they are over-determined for systems with more than two atoms. Thus, an alternative definition is necessary. Diabatic states are often defined as a state that retains certain key properties when the system moves along the reaction coordinate. For example, the generalized Mulliken-Hush scheme, a useful method for for electron transfer, retains the dipole moment in the diabatic states. The fragment excitation difference scheme is a similar method for energy transfer problems, in which the excitation population is localized to each fragment.

With a singlet exciton split into two triplet excitons, singlet fission has a great potential to increase the efficiency of solar cells. The Fragment Spin Difference (FSD) scheme was generalized to calculate the singlet fission coupling. Without manually including the CT components, the largest coupling strength obtained was 14.8 meV for two pentacenes in a crystal structure, or 33.7 meV for a transition-state structure, which yielded singlet fission lifetime of 239 or 37 fs, generally consistent to experimental result (80 fs). We found that the charge on one fragment in the S1 diabatic state correlates well with FSD coupling, indicating the importance of the CT component. The FSD approach is a useful first-principle method for singlet fission coupling, without the need to include the CT component explicitly. Further implementation for spin-completeness or a Restrictive Active Space (RAS) excitation improves the quality of excited states. The results predict well for a set of experimentally studied intramolecular singlet fission and triplet-triplet annihilation rates.

Heisenberg-scaled magnetometer with dipolar spin-1 condensates

Su Yi

We propose a scheme to realize a Heisenberg-scaled magnetometer using dipolar spin-1 condensates. The input state of magnetometer is prepared by slowly sweeping a transverse magnetic field to zero, which yields a highly entangled spin state of N atoms. We show that this process is protected by a parity symmetry such that the state preparation time is within the reach of the current experiment. We also propose a parity measurement with a Stern-Gerlach apparatus which is shown to approach the optimal measurement in the large atom number limit. Finally, we show that the phase estimation sensitivity of the proposed scheme roughly follows the Heisenberg scaling.

Topological states and cotranslational symmetry in strongly interacting systems

Chaohong Lee

It is still an outstanding challenge to characterize and understand thetopological features of strongly interacting states (such as bound states) in interactingquantum systems. Here, by introducing the cotranslational symmetry in an interactingmultiparticle quantum system, we develop a method to define a Cherninvariant, which is a generalization of the well-known Thouless-Kohmoto-NightingaledenNijs invariant, for identifying strongly interacting topological states. By using this topological invariant associated with the cotranslational symmetry, we explore several novelmultiparticle topological states in strongly interacting systems, such as,(i) topological magnon bounds states in ageneralized two-dimensional HeisenbergXXZ model, (ii) topological magnon bound states in a periodically modulated one-dimensional Heisenberg XXZ chains, and (iii) Thouless pumping in aninteracting Rice-Mele model of bosons.Our results not only provide a new approach to defining a topological invariantfor interacting multi-particle systems, but also give insights into the characterizationand understanding of strongly interacting topological states.

Strong coupling between a cavity and a half open space via a superconducting artificial atom

Zhihui Peng

We use a superconducting artificial atom simultaneously strongly coupled to a cavity and a half open space in experiment. With the special architecture, we study a vacuum induced Aulter-Townes doublet in the superconducting artificial atom. The Aulter-Townes splitting is observed in the reflection spectrum of the three-level atom when the transition between two excited states is resonant with the resonator. By varying an amplitude of the driving field applied to the resonator, we observe quantum-to-classical transition of the Aulter-Townes splitting. Our results may pave the way for the control of microwaves by single photons.

Molecular Characterization of (Oligothiophene)$_n$-tetracyanoquinodimethane Complexes (n = 1-5)

Sol Milena Mejía Chica*, Juan Carlos Salcedo Reyes** and Henry Alberto Méndez Pinzón**

Organic semiconductors (OSCs) are small conjugated molecules and polymers which currently play an important role in the rapidly growing field of optoelectronic devices. However, the use of OSCs in applications similar to those of inorganic semiconductors can only be realized through well-controlled electrical doping. In this sense, molecular electrical doping has emerged as a technique which allows a several orders of magnitude increase in the conductivity of OSCs by using small conjugated molecules as dopants. However, the detailed mechanism for molecular electrical doping is still a subject of discussion. Previous reported studies proposed a Hückel-like model, establishing the formation of charge transfer complexes (CPXs) acting as supramolecular dopants instead of an integer charge transfer between OSC and dopant, as is usually believed to occur. This study goes a step further, using DFT calculations to test the formation of charge transfer complexes based on the combination of OSC/dopant molecular pairs: oligothiophenes (1 to 5 monomers) doped with strong acceptors like tetracyanoquinodimethane (TCNQ) and its fluorinated derivatives (p-dopants). This work is focused on the influence of the oligothiophene size, the corresponding OSC ionization energies and the electron affinity of the dopant molecules on CPX formation. The main parameters analyzed are the shape and energy of the frontier molecular orbitals (HOMO-LUMO) of the isolated monomers, dopants and complexes. The calculations also provide Infrared and UV-VIS optical absorption spectra, geometric data, and topological parameters, the latter explaining the nature of the weak interactions that stabilize the complexes in agreement with the quantum molecular theory of Bader and collaborators. The most stable geometries for the complexes have also been found: molecular planes of OSC and dopants lying parallel each other, stabilized by weak interactions of moderate strength. The calculations agree closely with experimental data.

New Scenarios for Strongly Correlated Electrons

Wenjian Liu[a] and Mark R. Hoffmann[b]

According to when the static and dynamic components of electron correlation are treated, the available correlated wave function methods can be classified into three families, viz., "static-then-dynamic", "dynamic-then-static", and "static-dynamic-static (SDS)". In this lecture, I will discuss two novel approaches: (1) nonorthogonal state interaction (NOSI) of the "dynamic-then-static" family. Here, dynamic correlation (at any level of methodology) is first built into each individually optimized non-Aufbau model functions before the diagonalization in the space of nonorthogonal, dynamically correlated states is performed for static correlation; (2) *restricted* SDS, which employs *the same number* (Np) of primary, secondary and external states for describing the static, dynamic, and again static components of correlation. That is, the secular equation to be diagonalized is of dimension 3Np, irrespective of the numbers of correlated electrons and orbitals. Even the lowest-order realization of this seemingly *restricted* SDS framework, i.e., SDSPT2, is already very accurate for classic test problems of variable degeneracies, whereas a high-order realization, i.e., iCI (iterative Configuration Interaction), can converge monotonically and quickly to full CI from above, even when a rather poor reference is taken as the start. Time permitting, I will also highlight fundamental problems pertinent to relativistic explicitly correlated wave function methods.

QM and QM/MM Studies of Enzymatic Reactions: Mechanism and Selectivity

Rongzhen Liao

The understanding of the catalytic function of enzymes at an atomistic level is of both fundamental and practical interest. Quantum-chemical calculations have been shown to be a complement and alternative to experimental studies in elucidating the reaction mechanism of enzymes. In this talk, five examples will be presented, namely acetylene hydratase, formaldehyde ferredoxin oxidoreductase, benzoyl-CoA epoxidase, aldoxime dehydratase, fosfomycin resistance protein A and tetrachloroethylene reductive dechlorinase. For these enzymes, the calculations are able to rationalize the reactivity and explain the various selectivities, including chemoselectivity, regioselectivity, stereoselectivity, metal preference (W vs Mo), and oxidation state preference (Fe^{2+} vs Fe^{3+}).

The Dirac electron: physical consequences of deviations from whole numbers of the gyromagnetic factor, fine-structure constant, and gravitational invariant

Jean Maruani

The Dirac equation, which was derived by combining the relativistic invariance condition with the quantum probability principle, explained the half-integer spin of fermions and predicted antiparticles. In previous papers, we have conjectured that the electron is a massless charge spinning at light velocity in the positron field, this internal motion being responsible for the rest mass. The *wave beat* between the electron and the positron has been shown to be the reason for the gyromagnetic factor being g_e=2. Very accurate measurements and quantum electrodynamics computations have shown that actually g_e departs from 2 by:
$\delta_g \equiv (g_e - 2) / 2 \approx 0.001159652181 \approx 1/ 2a\pi + P/ 2(a\pi)^2 + A/ 2(a\pi)3 + \dots$ (within 1 ppb), a being the fine-structure constant inverse: $a \equiv \alpha^{-1} = \hbar c / k_e e^2$.

The fine-structure constant α was first introduced by Sommerfeld to express line splittings in atomic spectra. But its inverse was given its current significance by Eddington, who proposed the full integer value of 137 on theoretical grounds. The primeval prime number 137 is endowed with a number of special properties. However, the measured value of a departs from 137 by ~ 0.3 ppt: $\delta_a \equiv (a - 137) / 137 \approx 0.0002627664234$. In this paper, we propose an expansion of this increment similar to that derived for ge: $\delta_a \approx (1/2) (\pi /137)^2 - (9/16) (\pi /137)^4 \dots$ (within 0.4 ppb). A theoretical explanation is in progress.

Among the mathematical properties of 137 is a relation to the Mersenne Catalan series, $M_n = 2^n - 1$. The sequence of these numbers is: $M_2 = 3$, $M_3 = 7$, $M_7 = 127$, $M_{127} \approx 1.7014118 \times 10^{38}$. The sum of the first three terms is 137, which approximates the strength of the electromagnetic force. In previous papers, we have proposed equivalents of α to express the gravitational force, e.g.: $\delta_p = Gm_p^2 / \hbar c$. The inverse of this invariant: $d_p \equiv \delta_p^{-1} \approx 1.69328 \times 10^{38}$ (within 15 ppm due to the inaccuracy in G), appears very close to M_{127} ! The relative deviation: $\delta_d \equiv (M_{127} - d_p) / M_{127} \approx 0.00478021$, can be expanded in terms of 137 (as was δ_a) or of a (as δ_g): $\delta_d \approx (1/3) (2/137) - (2/5) (2/137)2 \dots$ (within 0.7 ppm) $\approx (2/ a\pi) + (5/ a\pi)^2 \dots$ (within 0.3 ppm).

The gravitational force F_g is related to the electromagnetic force F_e also in that F_g is to Fe as Fe is to the Planck force F_P: $F_g / aF_e = aF_e / F_P = 1 / d_p$, a and d_p being defined above. This is due to the fact that F_e is proportional to the square of the particle rest energy $E_0 = m_0 c^2$ expressed in terms of the much larger Planck energy: $(\hbar c/G)^{1/2}c$, while F_g is proportional to the fourth power of this ratio. All this comforts the Pythagorean view that physical constants are not due to chance, but determined by mathematical properties.

Relativity-Induced Bonding Picture Change in Heavy-Element Compounds

Jun Li

The Periodic Table (PT) of chemical elements is one of the most profound discoveries in chemistry. Each period row of PT corresponds to the filling of electrons in quantized shells. The elements in the same group column usually have similar properties due to the same electron configuration in their valence shell. While quantum mechanics alone accounts for all the periodic properties of the lighter elements, the case becomes more complicated for heavier elements roughly starting from the sixth row with so-called $6s^2$ inert electron pairs. Experimental and theoretical studies suggest that the mononuclear chemistry of Sg is rather similar to that of W and of Rg is similar to that of Au. Outside the immediate experimental availability, we here show a striking counterexample. The simplest dinuclear systems, the diatomic Sg_2 and Rg_2 molecules, are drastically different from their lightest congeners in terms of chemical bonding.

Quantum chemical calculations using wavefunction theory (WFT) and density functional theory (DFT) at the levels of PBE-DFT and *ab initio* CASSCF, $CASPT_2$, and CCSD(T) were carried out to optimize geometries and analyze the chemical bonding of M_2 (M = Cr, Mo, W, Sg) and A_2 (A = Cu, Ag, Au, Rg) molecules. He calculated Nalewajski-Mrozek bond orders are around 6 for Cr_2, Mo_2, W_2 and about 4 for Sg_2. Similarly, the ground state of Cu_2, Ag_2, Au_2 are shown to be singlet with s-s σ-bonding while Rg_2 has a triplet state with d-d σ-bonding. There exist significant differences between the superheavy-element molecules and their lighter congeners in the predicted electronic spectra and physiochemical properties.

Basis-set convergence in calculations with smooth Coulomb potentials

Cristina E. González-Espinoza, Paul W. Ayers and Andreas Savin

For molecular systems, solving the electronic Schödinger equation requires approximations for the two main components: 1) the wavefunction and 2) the Hamiltonian operator. For the wavefunction, one of the most common approximations is the use of a finite set of one-electron functions. Consequently, one has to choose a description of the N-electron system in the space of the chosen one-electron basis-set. The study of the basis-set limits of these approximations allows us to assess the accuracy of both, basis sets and N-electron models.

It is well known that the correct description of the correlation cusp requires a large number of one-electron basis functions with high angular momentum. Recently, we constructed two model potentials for the Coulomb interaction, which eliminate the singularity of the Coulomb potential while preserving the long-range asymptotic form of the potential. The use of a smooth potential permits the use of smaller basis sets, with fewer polarization functions. Here we provide a detailed study of the basis-set convergence of full configuration interaction (FCI) calculations using our model potential for the electron-electron interaction and optimized basis based on Dunning's correlation-consistent polarized basis sets.

Potential Energy Surfaces and Berry Phases beyond the Born-Oppenheimer Approximation: A New Perspective on Non-Aadiabatic Dynamics

Eberhard K.U. Gross

The starting point of essentially all modern electronic-structure techniques is the Born-Oppenheimer approximation. It not only makes calculations feasible, it also provides us with an intuitive picture of chemical reactions. Yet it is an approximation, and some of the most fascinating phenomena, such as photovoltaic dynamics, the process of vision, as well as phonon-driven superconductivity occur in the regime where the Born-Oppenheimer approximation breaks down. To tackle such situations one has to face the full Hamiltonian of the complete system of electrons and nuclei. We deduce an exact factorization of the full electron-nuclear wavefunction into a purely nuclear part and a many-electron wavefunction which parametrically depends on the nuclear configuration and which has the meaning of a conditional probability amplitude. The equations of motion for these wavefunctions lead to a unique definition of exact potential energy surfaces as well as exact geometric phases, both in the time-dependent and in the static case. We discuss a case where the exact Berry phase vanishes although there is a non-trivial Berry phase for the same system in Born-Oppenheimer approximation, implying that in this particular case the Born-Oppenheimer Berry phase is an artifact. In the time-domain, whenever there is a splitting of the nuclear wavepacket in the vicinity of an avoided crossing, the exact time-dependent surface shows a nearly discontinuous step. This makes the classical force on the nuclei jump from one to another adiabatic surface, reminiscent of Tully surface hopping algorithms. Based on this observation, we propose novel mixed-quantum-classical algorithms which provide a rather accurate, much improved over surface hopping, description of decoherence. This is demonstrated for the laser-induced ring opening of the oxirane molecule. We present a multi-component density functional theory that provides an avenue to make the fully coupled electron-nuclear system tractable in practice. Finally, we apply the concept of exact factorization to a purely electronic wave function, thereby separating, in a formally exact way, fast degrees of freedom (the core electrons) from slow degrees of freedom (electrons that ionize or produce harmonics). This allows us to deduce, in a controlled way, the so-called single-active-electron approximation and systematic improvements thereof.

Towards exotic quantum many-body physics on quantum simulator: Experimentally probing topological order and its breakdown

Xinhua Peng

The modern conception of phases of matter has undergone tremendous developments since the first observation of topologically ordered states in fractional quantum Hall systems in the 1980s. Topological phase not only plays a significant role in the basic scientific research of condensed matter physics, but also provides a natural medium for fault-tolerant quantum computation. Here, we explore the question: How much detail of the physics of topological orders can in principle be observed using state of the art technologies? We find that using surprisingly little data, namely the toric code Hamiltonian in the presence of generic disorders and detuning from its exactly solvable point, the modular matrices -- characterizing anyonic statistics that are some of the most fundamental finger prints of topological orders -- can be reconstructed with very good accuracy solely by experimental means. Using a kind of nuclear magnetic resonance simulator, we realize a first experimental demonstraton of these fundamental signatures of a topological order, a test of their robustness against perturbations, and a proof of principle -- that current technologies have attained the precision to identify phases of matter and, as such, probe an extended region of phase space around the soluble point before its breakdown. Given the special role of anyonic statistics in quantum computation, our work promises myriad applications both in probing and realistically harnessing these exotic phases of matter.

Rational Construction of Organic Composite Microwire/Microdisk Heterostructures for Controlled Output Coupling of Dual-Color Lasers

Wei Zhang

Dual-color lasers generated and outputted effectively at the nanoscale are crucial to constructing on-chip photonic circuits. Semiconductor Composite nanoheterostructures have emerged as a novel system to fabricate such ultracompact nanolasers, but remains a challenge to low-temperature solution assembly from traditional semiconductors due to intrinsic difficulties in achieving epitaxial growth of the mismatched materials. Organic dye molecules, with weak intermolecular interactions and good compatibility, are promising candidates for mildly preparing the dual-color nanoheterostructures for lasing. Here we design and construct a kind of organic microwire/microdisk interconnected dual-color heterostructures via a facile step-by-step liquid-phase assembly method. The process involves a facet-selective seeded-growth mechanism, where the nanowire nucleates and grows parallelly at the specific lateral edge of the microdisk with the assistance of the directional hydrogen-bonding interactions, resulting in the formation of nanowire-coupled microdisk heterojunctions. The microdisk therein can act as high-quality whispering-gallery-mode (WGM) microcavity for blue lasing, while the nanowire functions as the Fabry-Pérot (FP) resonator to deliver the green lasing. Moreover, the blue/green lasing can simultaneously generate and efficiently outcouple at the tip of nanowire, and the color/ratio can also be controllably modulated, providing a significant proof-of-concept trial for the flexible integration of microlasers with different colors for multi-band photonic application.

Absorption of microwave in driven superconducting artificial atoms

Yuxi Liu

In recent years, the research of superconducting artificial atoms has been made significant progress. Many phenomena in quantum optics have been demonstrated using superconducting quantum chips. In this talk, I will discuss how to realize electromagnetically induced transparency (EIT) and Aulter-Townes splitting (ATS) using three-level superconducting artificial atoms. I will introduce several new research results when the classical control field is changed to the quantum control field. In particular, I will show how to discern EIT and ATS spectra when the mean photon number of the quantum control field is changed from zero to the finite number.

Superheavy nuclei and new elements

Shangui Zhou

Atomic nuclei are finite quantum many-body systems consisting of nucleons, i.e., protons and neutrons. The exploration of charge and mass limits of atomic nuclei and the synthesis of long-lived or stable superheavy nuclei (SHN) are at the frontier of modern nuclear physics. In the 1960s, based on the stability due to quantum shell effects, the possible existence of an island of stability around $^{298}114$ was predicted. Such predictions advanced very much the construction of heavy ion accelerators and related detectors and the development of heavy ion physics. So far, elements with the proton number Z up to 118 have been synthesized via heavy ion fusion reactions in laboratories. Therefore the seventh period of the periodic table of elements is complete now. To synthesize even heavier elements or more neutron-rich SHN by using heavy ion fusion reactions, one confronts many challenges. More efforts should be made to study the properties of SHN both experimentally and theoretically. In this talk, the background, experimental status and challenges and recent progresses concerning the study of SHN will be presented.

Synthesis of *N*-Containing Heterocycles by Rh/Ag-Catalyzed Cycloaddition Reaction

Mingbo Zhou

This lecture mainly focuses on the construction of nitrogen-containing heterocyclic compounds, particularly seven-membered heterocyclic ring systems (azepine derivatives) and spiro[indene-1,2'-pyrrolidine] architectures by Rh/Ag-catalyzed cycloaddition reactions of alkynes with aziridines or their derivatives. These systems have broad substrate scope and allow the formation of multiple new chemical bonds in one step, leading to target ring systems with good yield and excellent regioselectivity. Moreover, these *N*-containing heterocycles are important skeletal units that are found in numerous natural products and in compounds with important chemical, biological, and medicinal properties.

Topological Dirac nodal lines in pure metal beryllium and its potential applications

Xingqiu Chen

Beryllium is a simple alkali earth metal, but has been the target of intensive studies for decades because of its unusual electron behaviors at surfaces. Puzzling aspects include (i) severe deviations from the description of the nearly free electron picture, (ii) anomalously large electron-phonon coupling effect, and (iii) giant Friedel oscillations. The underlying origins for such anomalous surface electron behaviors have been under active debate, but with no consensus. Here, by means of first-principles calculations, we discover that this pure metal system, surprisingly, harbors the Dirac node line (DNL) that in turn helps to rationalize many of the existing puzzles. The DNL is featured by a closed line consisting of linear band crossings and its induced topological surface band agrees well with previous photoemission spectroscopy observation on Be (0001) surface. We further reveal that each of the elemental alkali earth metals of Mg, Ca, and Sr also harbors the DNL, and speculate that the fascinating topological property of DNL naturally exist in other elemental metals as well.

Generalized Hirshfeld Atoms in Molecules

Paul W. Ayers

Many population analysis methods are based on the precept that molecules should be built from fragments (typically atoms) that maximally resemble the isolated fragment. The resulting molecular building blocks are intuitive (because they maximally resemble well-understood systems) and transferable (because if two molecular fragments both resemble an isolated fragment, they necessarily resemble each other). Information theory is one way to measure the deviation between molecular fragments and their isolated counterparts, and one that lends itself to analysis. We present key features, advantages, and disadvantages of the information-theoretic approach. Based on an extensive battery of computational tests, we present a generalization of Hirshfeld's atoms in molecules that has excellent mathematical and computational properties.

Complexes of Hyperguinones A and B with a Cu^{2+} Ion. A DFT Study

Liliana Mammino

Hyperguinones A and B are prenylated acylphloroglucinols differing only by the R chain in the COR group (ethyl and isopropyl respectively). A keto O is attached to one of the positions ortho to COR and the prenyl chain is attached to the next position. An OH is attached to the other positions ortho to COR, and a pyranoid ring is fused to the two following positions. They are found in *Hypericum* species and exhibit antioxidant activity. Complexes of these molecules with a Cu^{2+} ion were calculated at the DFT level, with the B3LYP functional, the 6-31+G(d,p) basis set for the light atoms and the LANL2DZ pseudopotential for the Cu^{2+} ion, considering all the sites to which Cu^{2+} might bind (including simultaneous coordination to two geometrically suitable sites). Complexes of a third structure, in which R is an isobutyl) were also calculated to obtain sufficient information for a comparative consideration of possible influences by the size and nature of R. The results show that the charge of the copper ion is reduced from +2 to +1 in the complexes, with an electron transfer from the molecule to the ion. The presentation includes consideration of the relative energies of the complexes, of the molecule-ion interaction energies, of the spin distribution in the complexes (highlighting the distribution of the unpaired electron in the molecule) and of the changes in the intramolecular hydrogen bonding patterns of the molecule caused by the complexation.

SATURDAY

Controlling the quantum states in adsorbed molecular magnets: First-principles based studies

Zheng Xiao

Precise control of quantum states in nanoscopic systems at atomic or molecular scale has opened a fascinating field, leading to potentially important applications in nanoelectronics, spintronics, quantum computation, photo-energy conversion, and heterogeneous catalysis. From the theoretical perspective, the relevant systems of experimental interest can be viewed as open quantum systems, in which the local electronic states couple with the surrounding material environment, which serves as the electron reservoir and thermal bath. Accurate characterization of open quantum system is thus the key to understanding the fascinating quantum mechanical features as well as their underlying mechanisms. However, this has remained rather challenging, especially for the evaluation of physical observables that are directly related to experimental measurements at a quantitative level. In this talk, I will present our recent efforts on the development of a hybrid approach, which combines the hierarchical equations of motion (HEOM) method with density functional theory (DFT) methods, to achieve first-principles based simulations of magnetic molecules in complex material environment.

Analytical Computation of Four-Electron Integrals for Extended Hylleraas-CI Wave Functions

Frank E. Harris

Hylleraas-CI (Hy-CI) is a superposition-of-configurations method of electronic structure calculation, with each wave-function term (configuration) constructed from a Slatertype orbital (STO) product to which is appended linearly at most one interelectron distance r_{ij}. This method was recently extended by the Nakatsuji group to include exponential correlation factors, calling this modification extended Hy-CI (E-Hy-CI). Some early Hy-CI computations expanded the STO′ s in terms of Gaussians, but the majority of the recent work directly used STO′ s. With STO′ s, formulas for the unlinked integrals (those not containing a product of type $r_{ij}r_{jk}/r_{ik}$) were published by Sims and Hagstrom in a series of papers of which the most recent was in 2015. Those authors also treated the linked integrals numerically by convergence-acceleration methods. Alternatively, one may evaluate the linked integrals using explicit, but complicated analytic formulas first derived by Remiddi and by Fromm and Hill. That work is summarized and extended in a contribution by the present author. Another method of unlinked integral evaluation using the r_{ij} as explicit coordinates was given by Ruiz in 2009 and in later papers, and Ruiz′ method was used by the Nakatsuji group to provide unlinked integrals for E-Hy-CI computations. The formulas of Sims, Hagstrom, and Ruiz did not yield simple formulas for the kinetic-energy integrals, and these integrals were not discussed by the Nakatsuji group. Recently the present author showed how the properties of vector spherical harmonics could be used to write kinetic-energy integrals in terms of those for the potential energy. The present contribution describes efforts to simplify and improve the numerical properties of E-Hy-CI computations. Three key elements of the approach presented here are (1) Use of the expansion of $e^{-\beta ij}/r_{ij}$ in terms of spherical harmonics of the angular coordinates of $\mathbf{r}_i$ and $\mathbf{r}_j$, a formula probably first used in quantum chemistry by Barnett and Coulson, (2) Use of an integration formula that avoids an explicit two-range integration, (3) Use of fixed-point arithmetic to force cancellation of equal but divergent terms.

Entanglement characteristics of bound and resonant few-body states

Anna Okopińska

Studying the physics of quantum correlations has gained increasing attention since the first experimental fabrication of artificial few-body systems on the nanoscale, such as semiconductor quantum dots or small ensembles of ultracold atoms in optical traps. Those structures may be considered as composed of a small number of interacting elements with controllable and highly tunable parameters, effectively described by Schrödinger equation. Performing analytical and numerical studies of simple models of few-body systems over a broad range of their parameters may provide a deeper understanding of correlation effects, especially in the neighborhood of critical points.

Bipartite correlations are well characterized by the entanglement spectrum, i.e. the eigenvalues of the reduced density matrix of the system partitioned into two subsystems. Entropies of entanglement spectrum can be conveniently used as correlation measures. I will study the entanglement spectrum of different few-body systems where the interactions depend on various powers of the distance between the constituents. Both closed and open systems will be considered. The linear entropy and von Neumann entropy will be discussed in dependence on the interaction type and strength. Particular attention will be paid to the behavior of entanglement on the border between the regimes of bound and resonant states.

Quantum Mechanics 100 Years of Mystery is Solved!

Akitomo Tachibana

In the theoretical study on the application of quantum electrodynamics (QED), recent research progress has led to solve the mystery (as Feynman said) involved in the foundation of quantum mechanics.

QED is a relativistic quantum field theory, a quantum theory of photons with electrons, and is considered the most successful accurate theory we have, e.g., to explain the Lamb shift, the anomalous magnetic moment of electron, and so on using the Feynman diagram technique of the covariant perturbation approach. We shall elaborate the non-perturbation approach in this talk.

This talk presents new aspects of QED from basic physics to physical chemistry with mathematical rigor. Topics covered include spin dynamics, chemical reactivity, the dual Cauchy problem, and more. Audience interested in modern applications of quantum field theory in nano-, bio-, and open systems will enjoy learning how the up-to-date quantum theory of radiation with matter works in the world of QED. In particular, chemical ideas restricted now to nonrelativistic quantum theory are shown to be unified and extended to relativistic quantum field theory that is basic to particle physics and cosmology: realization of the new-generation quantum theory.

Ultraviolet Nonlinear Optical effects in Black Phosphorus Quantum Dots

Jun He

As a new member of two-dimensional materials, black phosphorus (BP) has attracted unprecedented attention owing to its unique electronic and optoelectronic properties. In this work, a facile liquid exfoliation method was used to prepare BP nanosheets and BP Quantum Dots (QDs) suspended in NMP solvent. The Z-scan and pump-probe measurements indicated that BP nanosheets and QDs exhibit typical broadband saturable absorption properties. For BP nanosheets, an ultrafast recovery time (~50fs) and slow electron-hole recombination time (~1.9ps) of BP nanosheets were determined at 1550nm and correlated with intraband relaxation and interband carrier recombination, respectively. For BP QDs, the ultraviolet intraband relaxation time may be too short to be resolved, while the extracted interband relaxation time was 200~300 fs. The carrier diffusion length of 5 nm was obtained based on non-equilibrium carriers diffusion theory, which is consistent with the size of BP QDs. The excellent nonlinear optical characteristics of BP nanosheets and QDs may lead to new applications in lasers and optical switching.
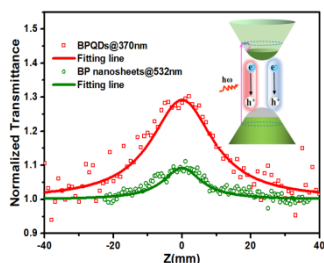

Figure 1.Open-aperture Z-scan of BPQDs/Nanosheets suspension at different excitation conditions；schematic diagram of intraband relaxation and interband recombination process for photoexcited carriers.
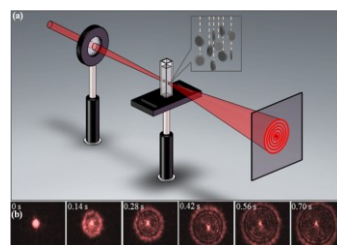

Figure 2. (a) Experimental setup and scenario of "wind-chime" model. (b) Snapshots of SSPM pattern formation.

SATURDAY

Abstracts of the Posters

P-001   **Constructing Arbitrary Multideterminant Wavefunctions**

Taewon D. Kim

Wavefunctions provide insight beyond those possible with the classical picture and are crucial for deciphering complex chemical phenomena, such as the stability of transition metals and reaction mechanisms involving catalysts. However, the exact wavefunctions are too expensive to compute except for small model systems. The goal of *ab initio* method development in quantum chemistry is to find the approximations to the exact wavefunction that reduce the computation cost without compromising accuracy. Recently, we have developed a general ansatz called Flexible Ansatz for N-electron Configuration Interaction (FANCI) that can construct any multideterminant wavefunctions. This ansatz is a generalization of the Configuration Interaction (CI) wavefunction, where the coefficients are parameterized by a weight function. By changing this function, we can reproduce popular wavefunction structures, such as CI, Coupled-Cluster, Tensor Product States (TPS), and geminal wavefunctions. The FANCI framework has been implemented as an open-source Python package, and we can easily construct and optimize arbitrary multideterminant wavefunctions. Here, we will discuss the structures of the FANCI framework and its implications on wavefunction properties, particularly the accuracy, cost and size-consistency.   We demonstrate the flexibility of this framework by constructing popular wavefunctions and modifying them to construct novel wavefunctions. We aim to show that the FANCI structures can serve as a powerful framework for ansatz development.

P-002   **Transition State Search and Geometry Optimization**

Xiaotian Derrick Yang and Paul W. Ayers

Geometry optimization is the key step in the computational modelling of chemical reactions. One cannot resolve the electronic energy of the reactant and product without accurately determining the structures. To efficiently locate the transition state(TS) structure of a chemical reaction, we developed a new method to construct initial guess was developed based on internal coordinates interpolation method.

Usually, internal coordinates (interatomic distances, angles, and torsions) are used for geometry optimization because these coordinates provide an intuitive representation of geometric structures. However, the redundancy leads to slow convergence and ill-defined torsion/dihedral angles. To circumvent this problem, a set of non-redundant coordinates, reduced internal coordinates, was introduced. The performance of these new coordinates for representing molecular structure changes was explored, and sophisticated quasi-newton optimization methods and trust radius methods for optimizing reduced internal coordinates were proposed and tested. All these methods will be included in the upcoming version of quantum chemistry package *HORTON*.

P-003   **A tree tensor method for the simultaneous determination of multiple eigenstates**

Yi Zhao[1], Paul W. Ayers[1], and C. Third[2]

In the field of photochemistry, transition metal, rare earth compound or temperature e_ects on molecular magnets , where many electronic states are needed or it contain strong correlation. A balance between accurate and calculation cost should be take into consideration. Here we propose a method to solve many excited states at once by using tree tensor structure. For FCI wavefunction, each basis depend on only single orbital Φ_{i_c} (q_c).

Instead of using Φ_{i_c} (q_c) that depend on single electon, we design function Φ_{i_w} ($\mathbf{q}_w$) depend on several orbitals and form a new basis by them. Each basis function for the node is a sum of product (SOP) of the basis function of its children in layer *l*-1.

$$(2)$$

By using a hievarchical basis in to tree tensor structure, the wavefunction is represented in a hierarchical CP-format. Followed with configuration interaction in this basis to solve for multiple excited states so that the accuracy and speed of the calculation be significantly improved.

POSTERS

P-004   **Procrustes, A Python Package for Matrix Similarity Computation**

Fanwang Meng

Procrustes analysis is concerned with matching two, or more, congurations of points. The term of Procrustes was put forward by Hurley JR and Catell RB at University of Illinois, which named after the ancient Greek mythological innkeeper, who brutally matched his guests to his special bed (stretching them or lopping off limbs). Here we show the python package for different kinds Procrustes analysis, orthogonal, permutation, symmetric and some two sided Procrustes with one transformation problems. Some examples were also given to show how this package works.

P-005   **Research on the Isotopic Effect of the Carboxylation by RuBisCO Using Free Energy Analysis**

Tianlong Jiang[1], Kenta Moriwaki[1], Osamu Kobayashi[2], Sebastian O. Danielache[1], Shinkoh Nanbu[1]

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-006   **Geometry-dependent band shift and dielectric modification of nanoporous Si nanowires**

Wangbing Yu

In order to obtain a detailed understanding of the modulation of electronic properties in nanoporous Si (np-Si) nanowires with containing ordered, nanometer-sized cylindrical pores, we propose a theoretical method to clarify the band shift and associated with the dielectric modification determined by the geometrical parameters, including nanowire diameter, pore size, pore spacing and porosity, based on size-dependent surface energy and atomic-bond-relaxation correlation mechanism. Our results reveal that the self-equilibrium strain induced by the atoms located at inner and outer surfaces with high coordination number imperfection and elastic interaction among pores in np-Si nanowires plays a dominant role in the band shift and dielectric depression. The tunable electronic properties of np-Si nanowires with negative curvature make them attractive for electronic and optoelectronic applications.

P-007   **Complementarity via error-free measurement in a two-path interferometer**

Yanjun Liu, Jing Lu and Lan Zhou[*]

We study both wave-like behavior and particle-like behavior in a general Mach–Zehnder interferometer with an asymmetric beam splitter. An error-free measurement in the detector is used to extract the which-path information. The fringe visibility V and the which-path information Ipath are derived, their complementary relation V + Ipath $\leq$ 1 is found, and the condition for the equality is also presented.

POSTERS

P-008   First-principles calculations of strength and ductility of magnesium by solid solutes

Ziran Liu

Electron work function (EWF) is a simple and fundamental parameter which largely reflects or characterizes the behavior of electrons in metals. This parameter can be used to guide the selection of solutes for effective modification of mechanical properties of Mg, an important metal for lightweight materials. From our prediction, adding solutes with EWFs lower than that of Mg can improve both strength and ductility of Mg, while adding elements with higher EWFs results in higher strength but lowered ductility. This study reveals the electronic origin of such influences of solutes on the strength and ductility of Mg and suggests an EWF-based principle or law for selecting appropriate solutes to achieve the optimal combination of strength and ductility for advanced Mg alloy.

P-009   Size-Tunable Band Alignment and Photovoltaic Conversion of MoS_2/WSe_2 van der Waals Heterostructures

Yipeng Zhao and Gang Ouyang

Two-dimensional transition metal dichalcogenides (TMDCs) and based heterostructures flaunt several fascinating properties that can address emerging market of energy conversion and storage devices. TMDC monolayers are direct-bandgap semiconductors in range of 1-2 eV with remarkably strong light-matter interactions, making it an important candidate for photovoltaic material. In addition, the elimination of surface dangling bonds is beneficial to form van der Waals heterostructures composed by different TMDCs despite the lattice mismatch. Ultrathin solar cell comprising of MoS_2/WS_2 bilayers can attain power conversion efficiency (PCE) of 1%, corresponding to approximately 1-3 orders of magnitude higher power densities than the traditional ultrathin solar cells. The solar cells consisting of stacked MoS_2 and WSe_2 monolayers form a type II van der Waals heterojunction and exhibit a PCE of 0.2%. Furthermore, simulation on atomically thin MoS_2/WSe_2 vertical heterojunction indicates the PCE of 1.13%. The high light absorption and impressive PCE of TMDC heterostructures make them promising candidates for ultrathin photovoltaic devices.

In spite of several achievements on band alignment and photovoltaic conversion of van der Waals heterostructures have been obtained, a systematic study to illustrate the size dependence of photoelectric properties from the perspective of atomistic origin is still lacking, and the relevant physical mechanism is still ambiguous. For example, how to quantify the effect of band alignment and band offset of TMDC heterostructures on carrier recombination, and how to realize the optimized PCE remain unclear. Therefore, in this study, we put forward an analytical method to address the band alignment and solar conversion efficiency of TMDC van der Waals heterostructures in terms of atomic-bond-relaxation correlation mechanism and detailed balance principle. Our results shown in Figure 1 indicate that the efficiency of monolayer MoS_2/WSe_2 is ~1.70%, and the efficiency of MoS_2/WSe_2 van der Waals heterostructures increases with thickness due to increasing optical absorption. Moreover, the underlying mechanism is clarified in Figure 2. Our method provides a reliable and useful way for gaining insight into the van der Waals heterostructures charge transport and photoelectric properties, such as recombination rate, photo-generated carriers, short circuit current, open-circuit voltage and conversion efficiency. Moreover, the results are validated by comparing them with the available evidence, providing the realistic efficiency targets and design principles.

POSTERS

P-016   **Interface effect on thermal boundary resistance and phonon thermal conductivity in Si/Ge core-shell nanowires**

Liang Zhang and Gang Ouyang

Heat transfer through interface attracts much attention in these years. The existence of interface between two dissimilar materials overheats nanoelectronics and impacts heat transfer greatly. It is a challenge how to modulate interface to tailor the thermal transport properties in nanodevices. However, many experimental and theoretical works have been made to explore the thermal boundary resistance (TBR) as well as the relationship between TBR and thermal transportations during the past decades. Until now, it is still not very clear that what the physical mechanism is, such as, how size effect influences the microscopic parameters (bonding energy, e.g.) and further thermal transportation properties; how surface/interface conditions (specular degree, e.g.) affects the TBR as well as thermal conductivity (TC) in nanoheterostructures. In this study, in terms of atomic-bond-relation correlation mechanism, we consider how size and interface strain affect TBR as well as phonon TC of Si/Ge core-shell nanowires (CSNWs) using a kinetic formula. It was found that Si core or Ge shell thickness, surface roughness and interface strain play key roles in modulating TBR as well as TC in Si/Ge CSNWs. Fig. 1 (a) and (b) are the TC and TBR of Si/Ge CSNWs as a function of Si core concentration (percentage of core area to cross-section area) with a fixed cross section 11×11-unit cells, respectively. Here P_1=0.97, P_2=0.5. We can see that the TC decreases firstly and then increases with increasing Si core concentration, thus has a much lower value than that in pristine Si or Ge nanowires. On the contrary, TBR enhances at first and then drops with increasing Si core concentration from 0 to 1. At the meantime, there is a peak when Si core concentration reaches about two-thirds. Both phonon velocities of the core and shells determine TBR. When Si core concentration increases and Ge shell concentration decreases, mean phonon velocity of the core increases from 0 and phonon velocity of the shells decreases from the value of that in pristine Ge. The rate of rise for phonon velocity of the core is larger at first and then smaller than rate of decline for phonon velocity of the shells. TBR rises at first and then drops, thus accounting for the existence of a peak in Fig. 1 (b). On the other hand, besides strong phonon-boundary scattering in nanosize, the existence of TBR can also enhance phonon-interface scattering, block phonon transportation and suppress phonon TC in Si/Ge CSNWs, thus accounts for the existence of a minimum in Fig. 1 (a). This may put a way to modulate interface thermal transportation in Si/Ge CSNWs. Significant decrease in TC with respect to bulk TC of materials and pristine nanowires proves that employing core–shell architectures for other possible thermoelectric material candidates would serve valuable opportunities to achieve a better thermoelectric performance.

P-018   ***Ab initio* Calculations for the Strain Modulation of Electronic Properties of Monolayer Black Phosphorus**

Zhe Zhang and Gang Ouyang

Recent advances in the fabrication of monolayer black phosphorus (MBP) call for a detailed understanding of the physics underlying the electronic structure and related modulation by the method of strain engineering. Herein, we present an analytic study to explore the uniaxial strain effect of band structure in MBP based on first-principles calculations and atomic-bond-relaxation correlation mechanism. The results from *ab initio* calculations show that the electronic band structure of MBP can be modulated by strain, which can further change the size and type of bandgap (see red dots in Figure 1). The change of bandgap in the *x* direction is also described in the Figure 1a. We found that the bandgap decreases monotonically with increasing compression strain from the value of 0.87 eV for the initial relaxed structure and reduces up to 0.76 eV at ε_x = -5% , while the bandgap increases with tensile strain from original relaxed structure and comes to the maximum value of 0.92 eV at ε_x = 3%, then reduces fleetly with larger tensile strain and drops to 0.86 eV at ε_x = 5%. The change of bandgap in the *y* direction is shown in the Figure 1b. Evidently, the bandgap decreases monotonically with increasing compression strain, while the bandgap increases with tensile strain from initial relaxed structure and reaches to 1.18 eV at ε_y = 5%. Moreover, we establish an analytic method and the predictions are shown the bandgap of MBP as a function of strain (see blue lines in Figure 1). The relaxations of bond length and bond angle which induced by tensile strain play a significant role in the band properties. The underlying mechanism on the strain-dependent band offset can be attributed to the variation of crystal potential induced by the changes of bond length, strength and angle, providing a better understanding of the modulation of electronic properties with strain engineering.

POSTERS

P-019   **Systematic study of the mechanism of super-heavy nuclei synthesis**

Xiaojun Bao

The superheavy nuclear production mechanism can be described by fusion reactions with the dinuclear system concept, and in the concept the deformations of the two nuclei are always assumed to stay at their ground state, and there are nucleons transferring between them. Actually the two nuclei have to deform due to very strong nuclear and Coulomb interactions between them. These deformations can be described by a Fokker-Planck equation analytically, and by combining them with a master equation, which describes the nucleon transfer between nuclei, the superheavy nuclear production cross sections are investigated systematically. The calculated results are in good agreement with available data.With the dinuclear system concept, and by taking the hexadecupole deformation in to consideration in addition to the quadrupole deformation, the hot fusion probability leading to the synthesis of SHN is investigated systematically. The dependence of the evaporation residue cross section (ERCS) to produce superheavy nuclei (SHN) on the isospin of colliding nuclei is analysed within the dinuclear system (DNS) concept. The ERCSs are discussed in detail and compared with existing experimental data. The fusion probabilities and surviving probabilities depend sensitively on the neutron numbers of the target and projectile nuclei. The prospects for the synthesis of superheavy nuclei (SHN) using radioactive beams are evaluated quantitatively within the framework of a dinuclear system (DNS) concept. In the most of cases the intensities of radioactive beams are significantly less than those of the stable beams, therefore using stable beam is predicted to be the most favorable method for producing SHN. In order to find a way which to produce superheavy nuclei (SHN), which appear in the gap between the SHN synthesized by cold fusion and those by hot fusion, or those so far have not yet been produced in the laboratory, we tried to make use of a set of projectile isotopic chain, to use radioactive beam projectile, and to test symmetric fusion reactions for gaining more neutrons to synthesize neutron richer SHN based on the DNS model via cold fusion reactions.

P-020   **Insights into the All-Metal $[Sb_3Au_3Sb_3]^{3-}$ Sandwich Complex from a QTAIM and Stress Tensor Analysis**

Lingling Wang[a], Yang Ping[a], Roya Momen[a], Alireza Azizi[a], Tianlv Xu[a], Juan I. Rodríguez[b], James S. M. Anderson[c,d], Steven R. Kirk[a*] and Samantha Jenkins[a*]

A QTAIM investigation of the $[Sb_3Au_3Sb_3]^{3-}$ sandwich complex is consistent with a previous investigation and reveals all of the bond critical points (*BCP*s) to be closed-shell *BCP*s with a degree of covalent character. All of the Sb--Au *BCP*s and Sb--Sb *BCP*s are found to possess metallicity. From the stress tensor analysis, a topological instability in the Sb--Au *BCP*s and Sb--Sb *BCP*s is revealed highlighting the need for an improved charge density. The topological instability is removed by using the SR-ZORA method to describe relativistic effects.

P-021   **QTAIM and Stress Tensor Characterization of Intramolecular Interactions Along Dynamics Trajectories of a Light-Driven Rotary Molecular Motor**

Lingling Wang, Guo Huan, Roya Momen, Alireza Azizi, Tianlv Xu, Steven R. Kirk,* Michael Filatov,*and Samantha Jenkins*

A quantum theory of atoms in molecules (QTAIM) and stress tensor analysis was applied to analyze intramolecular interactions influencing the photoisomerization dynamics of a light-driven rotary molecular motor. For selected nonadiabatic molecular dynamics trajectories characterized by markedly different S_1 state lifetimes, the electron densities were obtained using the ensemble density functional theory method. The analysis revealed that torsional motion of the molecular motor blades from the Franck−Condon point to the S_1 energy minimum and the S_1/S_0 conical intersection is controlled by two factors: greater numbers of intramolecular bonds before the hop-time and unusually strongly coupled bonds between the atoms of the rotor and the stator blades. This results in the effective stalling of the progress along the torsional path for an extended period of time. This finding suggests a possibility of chemical tuning of the speed of photoisomerization of molecular motors and related molecular switches by reshaping their molecular backbones to decrease or increase the degree of coupling and numbers of intramolecular bond critical points as revealed by the QTAIM/stress tensor analysis of the electron density. Additionally, the stress tensor scalar and vector analysis was found to provide new methods to follow the trajectories, and from this, new insight was gained into the behavior of the S_1 state in the vicinity of the conical intersection.

POSTERS

P-022   Exploration of the Forbidden Regions of the Ramachandran Plot (Φ-ψ) with QTAIM

*Roya Momen[1], Alireza Azizi[1], Lingling Wang [1], Yang Ping [1], Tianlv Xu[1], Steven R. Kirk[*1], Wenxuan Li[2], Sergei Manzhos[2] and Samantha Jenkins[*1]*

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 glycine amino acid monomer compared with 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 why the glycine amino acid monomer largely occupies the 'forbidden' region 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-023   Isomerization of the RPSB chromophore in the gas phase along the torsional pathways using QTAIM

*Ping Yang, Tianlv Xu, Roya Momen, Alireza Azizi, Steven R. Kirk *, Michael Filatov *, Samantha Jenkins ***

A QTAIM investigation of the torsion in both the clockwise and counter-clockwise directions about the π bonds of the retinal protonated Schiff base chromophore in the lowest electronically excited state provided a detailed description of the changing bonding topology that was sensitive to both the torsion and the direction of torsion. Analysis of the separate torsion calculations demonstrated a clear order of preferred bonding torsion in terms of principles of maximizing bonding. Unusual behavior of the bond ellipticity in the S_1 state was found for the two less favorable bonds for torsion and explained in terms of the presence of weak bonding interactions.

P-024   Fatigue and Photochromism S_1 Excited State Reactivity of Diarylethenes from QTAIM and the Stress Tensor

Ping Yang, Tianlv Xu, Roya Momen, Alireza Azizi, Steven R. Kirk[*], and Samantha Jenkins[*]

The realization of technologically relevant functional systems from idealized photochromic compounds remains elusive due to the double requirement that such switches must possess both highly efficient photo-isomerization reactivity and extremely low fatigue over a large number of switching cycles. Nowadays, improvements of the switching properties in complex diarylethene structures are mainly attained on a "trial and error" basis through chemical substitutions aimed at tuning the chemical properties of the core of the diarylethene. Therefore, we present new guiding principles to analyze the first excited state reactivity of diarylethenes based on the Quantum Theory of Atoms in Molecules (QTAIM) including the stress tensor. This approach straightforwardly provides consistent theoretical justification to partner the already successful symmetric substitution patterns obtained from experiments. The guiding principles provided by QTAIM and stress tensor suggest more complex asymmetric patterns should be included for the systematic design of new technologically relevant functional compounds. The stress tensor trajectory $T_\sigma(s)$ analysis is used to characterize the photochromism reaction as reusable and the fatigue reaction as irreversible and find candidate sites for alteration by future experiment.

P-025   The normal modes of vibration of benzene from the trajectories of stress tensor eigenvector projection space

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A QTAIM and Stress tensor eigenvector projection U_σ space formalism has been used to provide a detailed description of the participation of each of the bonds of the four infrared active normal modes of benzene. Analysis of the maximum U_σ space trajectory projections revealed a mixture of C-C and C-H bonding characteristics. The four-infrared active U_σ space trajectories were found to be unique. The normal mode with the highest infrared intensity was the only mode with non-zero maximum U_σ space trajectory projections in the most preferred and least preferred directions for the C-C and C-H bond critical points respectively.

POSTERS

P-027   Distinguishing and Quantifying the Torquoselectivity in Competitive Ring-Opening Reactions Using the Stress Tensor and QTAIM

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Currently the theories to explain and predict the classification of the electronic reorganization due to the torquoselectivity of a ring-opening reaction cannot accommodate the directional character of the reaction pathway; the torquoselectivity is a type of stereoselectivity and therefore is dependent on the pathway. Therefore, in this investigation we introduced new measures from quantum theory of atoms in molecules and the stress tensor to clearly distinguish and quantify the transition states of the inward (TSIC) and outward (TSOC) conrotations of competitive ring-opening reactions of 3-(trifluoromethyl)cyclobut-1-ene and 1-cyano-1-methylcyclobutene. We find the metallicity (r_b) of the ring-opening bond does not occur exactly at the transition state in agreement with transition state theory. The vector-based stress tensor response β_σ was used to distinguish the effect of the CN, CH_3, and CF_3 groups on the TSIC and TSOC paths that was consistent with the ellipticity ε, the total local energy density $H(r_b)$ and the stress tensor stiffness . We determine the directional properties of the TSIC and TSOC ring-opening reactions by constructing a stress tensor   space with trajectories   with length l in real space, longer l correlated with the lowest density functional theory-evaluated total energy barrier and hence will be more thermodynamically favored.

P-028   Polymorph-Selective Assembly and Charge-Transfer Emissions of Organic Cocrystal Microstructures for Photonic Applications

Yong Liu

Organic cocrystals, a single-phase crystal material assembled from two or more different molecules through intermolecular non-covalent interactions, could exhibit distinct and unpredicted optoelectronic properties and applications based on multicomponent synergistic and collective effects, such as ambipolar charge transport, ferroelectrics and optical waveguide emissions, capturing wide attentions and research interests. However, rationally tailoring the cocrystal luminescence properties, particularly by controlling the mode of molecular packing (polymorph) instead of chemical alteration of the donor/acceptor molecules remains a great challenge, and meanwhile, the controlled synthesis of organic cocrystals with regular shapes is also very difficult due to the elusive understanding of polymorph co-crystal formation mechanism until now. Here we controllable prepare two organic cocrystal polymorphs with the same donor/acceptor stoichiometric ratio via a concentration-dependent liquid-phase self-assembly strategy. Two cocrystal polymorphs with the distinct 1D microribbon and 2D microplate morphologies were obtained by changing the solution concentration of donor and acceptor molecules, which show excellent 1D/2D optical waveguide emissions, respectively. Interestingly, the charge-transfer emissive dynamics of two types of cocrystal polymorphs are also very different, which urges us to further investigate and understand the relationship between the packing structures and photonic properties in this kind of cocrystal system. These results of controlling the material structures and photonic properties by modulating kinetic assembly process for fabricating different microstructures, would provide enlightenment for the development of tailor-made mini-sized devices for photonic integrated circuits.

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