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
Monday 16th October………………………………………………………1
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Scientific and Social Program of QSCP-XXII Back Cover
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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

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 Academy of Sciences, Beijing, China)
   Exotic hadrons near threshold
Keynote/Invited Talks

Wednesday, 18 October P.M  

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
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

Chair ed 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

Chair ed 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
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

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

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
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
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

Closing Ceremony
Saturday, 21 October P.M  
Hunan Room III

17:00 to 18:00  
See you at QSCP-XXIII!
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
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 $\Omega_c$ 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 $[\text{Sb}_3\text{Au}_3\text{Sb}_3]^{3-}$ sandwich complex from a QTAIM and stress tensor analysis
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 ($\Phi, \psi$) 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 Diarylenes 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
<table>
<thead>
<tr>
<th>Participants</th>
<th>List in alphabetical order</th>
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