



**QSCP** XXII  
2017



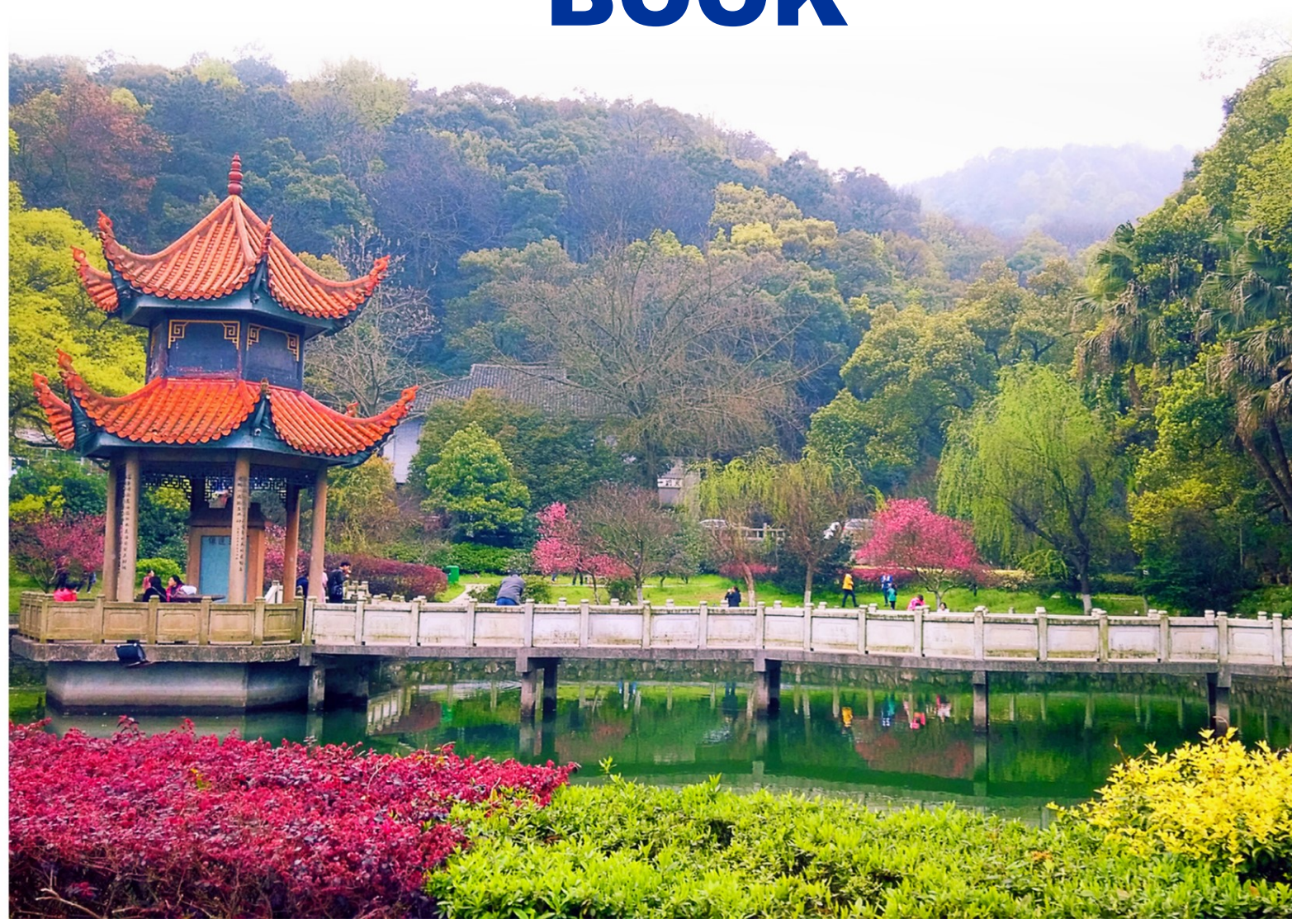
XXII International Workshop on

**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*

|                                                 |              |
|-------------------------------------------------|--------------|
| Monday 16th October.....                        | 1            |
| Tuesday 17th October.....                       | 2            |
| Wednesday 18th October.....                     | 4            |
| Thursday 19th October.....                      | 8            |
| Friday 20th October.....                        | 10           |
| Saturday 21th October.....                      | 12           |
| Poster Session: 20th October.....               | 14           |
| Abstracts of the Talks.....                     | 18           |
| Abstracts of the Posters.....                   | 45           |
| Participants List.....                          | 55           |
| Scientific and Social Program of QSCP-XXII..... | Back Cover   |
| Map of the venue.....                           | Inside Cover |

# **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

## ***Contact Information:***

Steven R. Kirk +86-151-1146-8042

Tianlv Xu +86-180-7316-9990



## 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<sub>1</sub>-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

MONDAY

---

## 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  $\text{Cq}^+$ -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

TUESDAY

---

## 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)

Halide 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

TUESDAY

---

## 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

WEDNESDAY

---

## 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

**Ruibao 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

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

WEDNESDAY

## 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

## 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

THURSDAY

---

## 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)

FRIDAY

*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-Adiabatic 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  $\text{Cu}^{2+}$  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

## Closing Ceremony

Saturday, 21 October P.M

Hunan Room III

---

17:00 to 18:00

See you at QSCP-XXIII!

SATURDAY

---

## 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 MoS<sub>2</sub>/WSe<sub>2</sub> 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 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



---

# Participants

List in alphabetical order

---

**Akitomo Tachibana**  
Kyoto University  
Kyoto  
Japan  
akitomo.tachibana99@gmail.com

**Artur F. Izmaylov**  
University of Toronto  
Toronto  
Canada  
artur.izmaylov@utoronto.ca

**Dahbia Talbi**  
University of Montpellier  
Montpellier  
France  
dahbia.talbi@umontpellier.fr

**Alain Dubois**  
CNRS, Université Pierre et Marie  
Curie  
Paris  
France  
alain.dubois@upmc.fr

**Benliang Zhou**  
Hunan Normal University  
Changsha  
China  
blzhou@hunnu.edu.cn

**Debashis Mukherjee**  
Indian Association for the  
Cultivation of Science  
Kolkata  
India  
pcdemu@gmail.com

**Alexander V. Glushkov**  
University of Odessa  
Odessa  
Ukraine  
glushkovav@gmail.com

**Chang Liu**  
Hunan Normal University  
Changsha  
China  
273115472@qq.com

**Eberhard K. U. Gross**  
Max Planck Institute of  
Microstructure Physics  
Halle (Saale)  
Germany  
hardy@mpi-halle.mpg.de

**Alia V. Tadjer**  
University of Sofia  
Sofia  
Bulgaria  
tadjer@chem.uni-sofia.bg

**Chao Kong**  
Hunan Normal University  
Changsha  
China  
819209843@qq.com

**Eric Suraud**  
University of Toulouse  
Toulouse  
France  
suraud@irsamc.ups-tlse.fr

**Alireza Azizi**  
Hunan Normal University  
Changsha  
China  
a\_azizi\_83@yahoo.com

**Chaohong Lee**  
Sun Yat-sen University  
Guangzhou  
China  
lichao2@mail.sysu.edu.cn

**Erkki J. Brändas**  
Uppsala University  
Uppsala  
Sweden  
erkki.brandas@gmail.com

**Andrey A. Svinarenko**  
University of Odessa  
Odessa  
Ukraine  
svinarenkoaa@gmail.com

**Chao-Ping Hsu**  
Academia Sinica  
Taipei  
Taiwan  
cherri@sinica.edu.tw

**Eugeniy V. Ternovsky**  
University of Odessa  
Odessa  
Ukraine  
ternovskyev@gmail.com

**Anlian Pan**  
Hunan University  
Changsha  
China  
Anlian.pan@hnu.edu.cn

**Congzhang Gao**  
Institute of Applied Physics and  
Computational Mathematics  
Beijing  
China  
czgao88@hotmail.com

**Fanwang Meng**  
McMaster University,  
Hamilton  
Canada  
fwmeng88@gmail.com

**Anna Okopińska**  
Jan Kochanowski University  
Kielce  
Poland  
okopin@ujk.edu.pl

**Cristina E Gonzalez Espinoza**  
McMaster University  
Hamilton  
Canada  
crisbeth46@gmail.com

**Frank E. Harris**  
University of Utah  
Salt Lake City  
USA  
harris@qtp.ufl.edu

**Gang Ouyang**

Hunan Normal University  
Changsha  
China  
gangouy@hunnu.edu.cn

**Jeng-Da Chai**

National Taiwan University  
Taipei  
Taiwan  
jdchai@phys.ntu.edu.tw

**Jun Li**

Tsinghua University  
Beijing  
China  
junli@tsinghua.edu.cn

**Georgi V. Vayssilov**

University of Sofia,  
Sofia  
Bulgaria  
gnv@chem.uni-sofia.bg

**Jhih-Wei Chu**

National Chiao Tung University  
Hsinchu  
Taiwan  
jwchu@g2.nctu.edu.tw

**Jun-ya Hasegawa**

Hokkaido University  
Hokkaido  
Japan  
hasegawa@cat.hokudai.ac.jp

**Hadieh Monajemi**

University of Malaya  
Kuala Lumpur  
Malaysia  
h.monajemi@hotmail.com

**J. Z. Hui Zhang**

New York University Shanghai  
Shanghai  
China  
john.zhang@nyu.edu

**Kailei Wang**

Hunan Normal University  
Changsha  
China  
869605900@qq.com

**He Xiao**

East China Normal University  
Shanghai  
China  
xiaoh@phy.ecnu.edu.cn

**Jean Maruani**

CMOA  
France  
marjema@wanadoo.fr

**Kaito Takahashi**

Academia Sinica,  
Taipei  
Taiwan  
kt@gate.sinica.edu.tw

**Herbert A. Früchtl**

University of St. Andrews  
St. Andrews  
U.K  
herbert.frucht1@st-andrews.ac.uk

**Jian Liu**

Peking University  
Beijing  
China  
jianliupku@pku.edu.cn

**Kwang S. Kim**

Ulsan National Institute of  
Science and Technology  
Ulsan  
South Korea  
kimks@unist.ac.kr

**Hui Dong**

Graduate School of Chinese  
Academy of Engineering Physics  
Beijing  
China  
hdong@gascaep.ac.cn

**Jianxin Song**

Hunan Normal University  
Changsha  
China  
jxsong@hunnu.edu.cn

**Leman Kuang**

Hunan Normal University  
Changsha  
China  
lmkuang@hunnu.edu.cn

**Hui Jing**

Hunan Normal University  
Changsha  
China  
jinghui73@foxmail.com

**Jieci Wang**

Hunan Normal University  
Changsha  
China  
jcwang@hunnu.edu.cn

**Liang Zhang**

Hunan Normal University  
Changsha  
China  
973917025@qq.com

**Hongrong Liu**

Hunan Normal University  
Changsha  
China  
hrliu@hunnu.edu.cn

**Jieqiao Liao**

Hunan Normal University  
Changsha  
China  
jqiao@hunnu.edu.cn

**Libin Fu**

Institute of Applied Physics  
and Computational  
Mathematics  
Beijing  
China  
lbfu@gascaep.ac.cn

**James S.M. Anderson**

The University of Tokyo  
Tokyo  
Japan  
james@tcl.t.u-tokyo.ac.jp

**Jun He**

Central South University  
Changsha  
China  
junhe@csu.edu.cn

**Liemao Cao**

Hunan Normal University  
Changsha  
China  
136355754@qq.com

**Liliana Mammino**  
University of Venda  
Venda  
South Africa  
sasdestria@yahoo.com

**Min Yu**  
Hunan Normal University  
Changsha  
China  
459952752@qq.com

**Paul W. Ayers**  
McMaster University  
Hamilton  
Canada  
ayers@mcmaster.ca

**Lingling Wang**  
Hunan Normal University  
Changsha  
China  
1139493940@qq.com

**Ming Lei**  
Beijing University of Chemical  
Technology  
Beijing  
China  
leim@mail.buct.edu.cn

**Peng Zhang**  
Renmin University of China  
Beijing  
China  
pengzhang@ruc.edu.cn

**Ling Xu**  
Hunan Normal University  
Changsha  
China  
xulingomchem@163.com

**Mingbo Zhou**  
Hunan Normal University  
Changsha  
China  
zhoumingbo@hunnu.edu.cn

**Ping Yang**  
Hunan Normal University  
Changsha  
China  
532484256@qq.com

**Mang Feng**  
Wuhan Institute of Physics and  
Mathematics  
Chinese Academy of Sciences  
China  
mangfeng@wipm.ac.cn

**Mingxing Chen**  
Hunan Normal University  
Changsha  
China  
mxchen@hunnu.edu.cn

**Pradeep R. Varadwaj**  
The University of Tokyo  
Tokyo  
Japan  
pradeep@tcl.t.u-tokyo.ac.jp

**Marco Nascimento**  
Federal University of Rio de Janeiro  
Rio de Janeiro  
Brazil  
chaer01@gmail.com

**Mingzhi Wang**  
Hunan Normal University  
Changsha  
China  
1026665397@qq.com

**Qiang Zhao**  
Institute of High Energy  
Physics,  
Chinese Academy of Sciences  
China  
zhaoq@ihep.ac.cn

**Marek J. Wojcik**  
Jagiellonian University  
Kraków  
Poland  
wojcik@chemia.uj.edu.pl

**Nadine Halberstadt**  
Universite Toulouse  
Toulouse  
France  
Nadine.Halberstadt@irsamc.ups-tlse.fr

**Qiyuan Pan**  
Hunan Normal University,  
Changsha,  
China  
panqiyuan@hunnu.edu.cn

**Masataka Nagaoka**  
Nagoya University  
Nagoya  
Japan  
mnagaoka@is.nagoya-u.ac.jp

**Nike Dattani**  
McMaster University  
Hamilton  
Canada  
dattani.nike@gmail.com

**Rongzhen Liao**  
Huazhong University of  
Science and Technology  
Wuhan,  
China  
rongzhen@hust.edu.cn

**Mengjie Wang**  
Hunan Normal University  
Changsha  
China  
mjwang@hunnu.edu.cn

**Olga Yu. Khetselius**  
University of Odessa  
Odessa  
Ukraine  
okhetsel@gmail.com

**Roya Momen**  
Hunan Normal University  
Changsha  
China  
r.momen24@yahoo.com

**Michael Filatov**  
Hunan Normal University,  
Changsha,  
China  
mike.filatov@gmail.com

**Paul A. Johnson**  
Université Laval  
Quebec  
Canada  
paul.johnson@chm.ulaval.ca

**Rudolph A. Marcus**  
California Institute of  
Technology  
California  
USA  
ram@caltech.edu

**Ruibo Wu**

Sun Yat-sen University  
Guangzhou  
China  
wurb3@mail.sysu.edu.cn

**Taewon D. Kim**

McMaster University  
Hamilton  
Canada  
kimt33@mcmaster.ca

**Wei Zhang**

Hunan Normal University  
Changsha  
China  
wzhang0222@hunnu.edu.cn

**Samantha Jenkins**

Hunan Normal University  
Changsha  
China  
samanthajsuman@gmail.com

**Tanja van Mourik**

University of St. Andrews  
St. Andrews  
UK  
tanja.vanmourik@st-andrews.ac.uk

**Weichang Zhou**

Hunan Normal University  
Changsha  
China  
wchangzhou@hunnu.edu.cn

**Shangui Zhou**

Institute of Theoretical Physics,  
Chinese Academy of Sciences  
Beijing  
China  
sgzhou@itp.ac.cn

**Tianlong Jiang**

Sophia University  
Tokyo  
Japan  
nostramemoria@eagle.sophia.ac.jp

**Wenjian Liu**

Peking University  
Beijing  
China  
liuwj@pku.edu.cn

**Shinkoh Nanbu**

University of Sophia  
Tokyo  
Japan  
shinkoh.nanbu@sophia.ac.jp

**Tianlv Xu**

Hunan Normal University  
Changsha  
China  
xutl@hunnu.edu.cn

**Xiao Zheng**

University of Science and  
Technology of China  
Beijing  
China  
xz58@ustc.edu.cn

**Sol M. Mejía**

Pontificia Universidad Javeriana  
Bogotá  
Colombia  
sol.mejia@javeriana.edu.co

**Valentin. B. Ternovsky**

University of Odessa  
Odessa  
Ukraine  
ternovskyvb@gmail.com

**Xiaoguang Wang**

Zhejiang University  
Hangzhou  
China  
xgwang1208@zju.edu.cn

**Songbai Chen**

Hunan Normal University  
Changsha  
China  
csb3752@hunnu.edu.cn

**Vasily V. Buyadzh**

University of Odessa  
Odessa  
Ukraine  
buyadzhiyv@gmail.com

**Xiaojun Bao**

Hunan Normal University  
Changsha  
China  
baoxiaojun@hunnu.edu.cn

**Steven R. Kirk**

Hunan Normal University  
Changsha  
China  
stevenrkirk@gmail.com

**Vladimir V. Tchernyi**

Modern Science Institute at SAIBR  
Moscow  
Russia  
chernyv@list.ru

**Xiaotian D. Yang**

McMaster University  
Hamilton  
Canada  
yxt1991@gmail.com

**Stijn Fias**

McMaster University  
Hamilton  
Canada  
fiass@mcmaster.ca

**Wangbin Yu**

Hunan Normal University  
Changsha  
China  
20172816@qq.com

**Xin Xu**

Fudan University  
Shanghai  
China  
xxchem@fudan.edu.cn

**Su Yi**

Institute of Theoretical Physics,  
Chinese Academy of Sciences  
China  
syi@itp.ac.cn

**Wangjun Lu**

Hunan Normal University,  
Changsha,  
China  
wangjun\_lu@sina.com

**Xingqiu Chen**

Institute of Metal Research,  
Chinese Academy of  
Sciences  
China  
xingqiu.chen@imr.ac.cn

**Xinhua Peng**

University of Science and  
Technology of China  
Beijing  
China  
xhpeng@ustc.edu.cn

**Yong Liu**

Hunan Normal University  
Changsha  
China  
liuyong0026@sina.com

**Xiongjun Fang**

Hunan Normal University  
Changsha  
China  
fangxj@hunnu.edu.cn

**Yong Pei**

Xiangtan University  
Xiangtan  
China  
ypnku78@gmail.com

**Xiongjun Liu**

Peking University  
Beijing  
China  
xiongjunliu@pku.edu.cn

**Youwen Long**

Institute of Physics,  
Chinese Academy of Sciences  
China  
ywlong@iphy.ac.cn

**YanJun Liu**

Hunan Normal University  
Changsha  
China  
liuyjhnu@163.com

**Yuehui Zhou**

Hunan Normal University  
Changsha  
China  
1743867008@qq.com

**Yasuteru Shigeta**

University of Tsukuba  
Tsukuba,  
Japan  
shigeta@ccs.tsukuba.ac.jp

**Yuxi Liu**

Tsinghua University  
Beijing  
China  
yuxiliu@tsinghua.edu.cn

**Yi Zhao**

Xiamen University  
Xiamen  
China  
yizhao@xmu.edu.cn

**Zhe Zhang**

Hunan Normal University  
Changsha  
China  
2357526108@qq.com

**Yibo Lei**

Northwest University  
Xi'an  
China  
leiyibo@163.com

**Zhihui Peng**

Hunan Normal University  
Changsha  
China  
zhihui.peng@hunnu.edu.cn

**Yilin Zhao**

McMaster University  
Hamilton  
Canada  
zhao229@mcmaster.ca

**Zhiqiang Gao**

National University of Singapore  
Singapore  
chmgaoz@nus.edu.sg

**Yipeng Zhao**

Hunan Normal University  
Changsha  
China  
1254900259@qq.com

**Ziran Liu**

Hunan Normal University  
Changsha,  
China  
zrlu@hunnu.edu.cn