International Conference on Theoretical and High Performance Computational Chemistry 2023

CONFERENCE GUIDE

23 - 26 November 2023

Haikou, China

	Thursday 23 November	Friday 24 November	Saturday 25 November	Sunday 26 November
Morning Session 8:30 - 12:30	———	**Opening** Chang-guo ZHAN Chenglong LI Chaoyuan ZHU Sponsor's Presentation ——— Zenghui ZHANG Yunpeng LU Ruibo WU	Guanhua CHEN Zexing CAO Yinglong MIAO **Poster Session** ——— Jing MA Zhenyang LIN Shuxian HU	**Symposium on Academic Exchange**
Lunch 12:30 - 14:00		Buffet	Buffet	Buffet
Afternoon Session 14:00 - 18:00	**Registration** 14:00 - 22:00	Yaoqi ZHOU Fang ZHENG Defang OUYANG Hao WANG ——— Shengyong YANG Yong LIANG Xueqing GONG Jin WEN	Xin XU Yiqin GAO Shuhua LI Feiwu CHEN ——— Qian PENG Wei HU Wenhao LIANG Zhe LI **Awards & Closing**	
Dinner 18:00 - 19:30	Buffet	Banquet	Buffet	

International Conference on Theoretical and High Performance Computational Chemistry 2023

(ICT-HPCC23)

1. Conference Information

a) Date: 23 - 26 November 2023

b) City: Haikou, China

c) Website: http://ict-hpcc.vlcc.cn/

d) Address: International Academic Exchange Center Hainan University

No. 58, Renmin Avenue, Meilan District, Haikou City, Hainan Province

(海南省海口市美兰区人民大道 58 号海南大学国际学术交流中心)

2. Conference Room

Level 2 Herong Hall (2 层和荣厅)

3. Meals

a) **Lunch**

November 24/25/26: 12:30-14:00, Level 1 Hexi Hall (1 层和熙厅)

b) **Dinner**

November 23/25: 18:00-19:30, Level 1 Hexi Hall (1 层和熙厅)

4. Poster Session

Date: November 25 09:45 ~ 10:45

Place: Level 2 Herong Hall (2 层和荣厅)

5. Contacts

Jing LI	010-58812172/ 13520969978
Baohua ZHANG	13581885294
Qian LIU	15201280496

6. Organizations

- **Chair**

❑ Chang-Guo ZHAN (University of Kentucky, USA)

- **Advisory Committee**

❑ Jun LI (Tsinghua University, China)

❑ Xiangyuan LI (Sichuan University, China)

❑ Wenjian LIU (Shandong University, China)

❑ Zhigang SHUAI (The Chinese University of Hong Kong, China)

❑ Jinlong YANG (University of Science and Technology of China, China)

- **Organizing Committee**

▲ **Chair**

❑ Xuebin CHI (Computer Network Information Center, CAS, China)

▲ **Secretary General**

❑ Zhong JIN (Computer Network Information Center, CAS, China)

❑ Haibin LUO (Hainan University)

7. Organizers & Sponsors

▲ **Organizers**

❑ Computer Network Information Center, Chinese Academy of Sciences

▲ **Co- Organizers**

❑ Hainan University

▲ **Sponsors**

❑ Bureau of International Cooperation, Chinese Academy of Sciences

❑ Inspur Technologies Co., Ltd

PROGRAM

Thursday, November 23

14:00 - 22:00	**Registration**	Level 1 Lobby
18:00 - 19:30	**Welcome Reception Dinner**	Level 1 Hexi Hall (1 层和熙厅)

Friday, November 24

8:30 - 9:00	**Opening**

Session 1

Session Chair	**Haibin LUO**	*Hainan University*
9:00 - 9:30	**Chang-guo ZHAN**	*University of Kentucky*
	Development of a Platform Technology for Treatment of Pain and Chronic Diseases via Computational Design	
9:30 - 9:55	**Chenglong LI**	*University of Florida*
	Elion: An Artificial Intelligence-based computational platform for drug discovery and optimization	
9:55 - 10:20	**Chaoyuan ZHU**	*South China Normal University*
	Nonadiabatic Molecular Dynamic Simulation with TDDFT Method for Complex Systems	
10:20 - 10:45	**Sponsor's Presentation**	
	Inspur Technologies Co., Ltd	
10:45 - 11:05	**Group Photo & Break**	

Session 2

Session Chair	**Shengyong YANG**	*Sichuan University*
11:05 - 11:30	**Zenghui ZHANG**	*New York University Shanghai*
	Protein Interaction systems: computation and application	
11:30 - 11:55	**Yunpeng LU**	*Nanyang Technological University*
	Graph Neural Networks and Transfer Learning for Oral Bioavailability Prediction	
11:55 - 12:20	**Ruibo WU**	*Sun Yat-sen University*
	Synergistic Data-Physical Models Driving the Prediction of Biosynthetic Pathways for Natural Products	
12:20 - 14:00	**Lunch**	Level 1 Hexi Hall (1 层和熙厅)

Session 3

Session Chair	**Chang-guo ZHAN**	*University of Kentucky*
14:00 - 14:25	**Yaoqi ZHOU**	*Shenzhen Bay Laboratory*
	Protein Design: the past, the present, and the future	
14:25 - 14:50	**Fang ZHENG**	*University of Kentucky*
	Development of enzyme therapies for treatment of cocaine use disorders through computational design	
14:50 - 15:15	**Defang OUYANG**	*University of Macau*
	Opportunity and challenge of artificial intelligence (AI) in drug delivery	
15:15 - 15:40	**Hao WANG**	*Shandong University*
	Enhanced Sampling for Rare Event Kinetics	
15:40 - 16:00	**Break**	

Session 4

Session Chair	**Chenglong LI**	*University of Florida*
16:00 - 16:25	**Shengyong YANG**	*Sichuan University*
	Molecular deep generative model and its applications in drug discovery	
16:25 - 16:50	**Yong LIANG**	*Nanjing University*
	DFT calculations guided design of new catalysts and reactions	
16:50 - 17:15	**Xueqing GONG**	*Shanghai Jiao Tong University*
	Comprehensive and Explainable Fragmentation: A Machine Learning Approach for Fast and Accurate EI-MS Peak Prediction	
17:15 - 17:40	**Jin WEN**	*Donghua University*
	Ultrafast Photochemical Dynamics Controlled by Light Fields	
18:30 - 20:30	**Banquet**	Jinshuimen Riverside Seafood Restaurant (18:00 海大东门集合)

Saturday, November 25

Session 5

Session Chair	**Shuhua LI**	*Nanjing University*
8:30 - 8:55	**Guanhua CHEN**	*The University of Hong Kong*
	Construct exchange-correlation functional via machine learning and delta-learning method	
8:55 - 9:20	**Zexing CAO**	*Xiamen University*
	Multiscale QM/MM Simulations of Enzyme Catalysis	
9:20 - 9:45	**Yinglong MIAO**	*University of North Carolina - Chapel Hill*
	Accelerated Molecular Dynamics and Drug Discovery	
9:45 - 10:45	**Break and Poster Session**	

Session 6

Session Chair	**Defang OUYANG**	*University of Macau*
10:45 - 11:10	**Jing MA**	*Nanjing University*
	Electronic Structure Properties and Solubility Predictions for Organic Molecules	
11:10 - 11:35	**Zhenyang LIN**	*The Hong Kong University of Science and Technology*
	Achieving Localization and Semi-localization via Orbital Alignment – Fragment Aligned Molecular Orbital Analysis	
11:35 - 12:00	**Shuxian HU**	*University of Science and Technology Beijing*
	Electronic Structure and properties of Plutonium Compounds	
12:00 - 14:00	**Lunch**	Level 1 Hexi Hall (1 层和熙厅)

Session 7

Session Chair	**Guanhua CHEN**	*The University of Hong Kong*
14:00 - 14:25	**Xin XU**	*Fudan University*
	A General Framework of Scanning Tunneling Microscopy Based on Bardeen's Approximation for Isolated Molecules	
14:25 - 14:50	**Yiqin GAO**	*Peking University*
	AI Powered Molecular Simulations	

14:50 - 15:15	**Shuhua LI**	*Nanjing University*
	Combined molecular dynamics and coordinate driving method for automatically searching complicated reaction pathways	
15:15 - 15:40	**Feiwu CHEN**	*University of Science and Technology Beijing*
	Block Effective Hamiltonian Theory and its Application	
15:40 - 15:55	**Break**	

Session 8

Session Chair	**Zexing CAO**	*Xiamen University*
15:55 - 16:20	**Qian PENG**	*Nankai University*
	Spin control on Iron-catalyzed reactions from the Computational Perspective	
16:20 - 16:45	**Wei HU**	*University of Science and Technology of China*
	High performance computing for first-principles Kohn-Sham density functional theory towards exascale supercomputers	
16:45 - 17:05	**Wenhao LIANG**	*Computer Network Information Center,CAS*
	Efficient Computing for Reduced Density Matrix on GPUs	
17:05 - 17:30	**Zhe LI**	*Sun Yat-sen University*
	Development of FEP method and its applications in drug discovery	
17:30 - 18:00	**Awards & Closing**	
18:00 - 19:30	**Dinner**	Level 1 Hexi Hall (1 层和熙厅)

Sunday, November 26

8:30 - 12:30	**Academic Exchange**	
	Workshop on Future Directions in Combining Theoretical Chemistry and High Performance Computing	
12:30 - 14:00	**Lunch**	Level 1 Hexi Hall (1 层和熙厅)

POSTER SESSION

Saturday, November 25, 09:45 ~ 10:45, Level 2 Herong Hall (2 层和荣厅)

P1 **Qiang REN**

Mesophase structure of needle coke and Effect of coking inhibitor on polymerization

P2 **Kefeng YAN**

Exploring Hydration mechanism of salt ions on the methane hydrate formation: Insights from experiments, QM calculations and MD simulations

P3 **Xianyang ZHANG**

Theoretical Insights into the Formation and Reactivity of Hydride on ZnO(1010) Surfaces

P4 **Yanping ZHANG**

Strategies to improve the oxygen reduction reaction activity on Pt-based electrocatalysts: A density functional theory study

P5 **Xi CHEN**

Unraveling the Allosteric Mechanisms of Prolyl Endopeptidases for Celiac Disease Therapy: Insights from Molecular Dynamics Simulations

P6 **Yafeng TIAN**

Computational Investigations on Reaction Mechanisms of the Covalent Inhibitors Ponatinib and Analogs Targeting the Extracellular Signal-Regulated Kinases

P7 **Jun YU**

QM/MM and MM MD Simulations on Enzymatic Degradation of the Nerve Agent VR by Phosphotriesterase

P8 **Xiaoyuan LIU**

Combination of multiple methods and views for recognition, transportation, and structure-guided modification of lysine-specific demethylase phenylcyclopropylamine inhibitor

P9 **Dongzhi LI**

Optimization and Rationalization of Palladium-Catalyzed Carbonylation Reaction Systems through Machine Learning

P10 **Zhaobin DING**

Machine-learning aided investigation of determining structural factors for oxygen reduction reaction activity of single-atomic catalysts

P11 **Nan LV**

AlphaTraj: A protein-pocket dynamics analysis software

P12 **Yuzhuang FU**

Coordination Dynamics of Iron Center Enables the C-H Bond Activation: QM/MM Insight into the Catalysis of Hydroxyglutarate Synthase (HglS)

P13 **Huangchao XU**

Deep learning-based classification model for GPR151 activator activity prediction

P14 **Mi ZHANG**

P15 **Yixuan Zhou**

Polymerization mechanism of aluminosilicate clusters：Ab initio molecular dynamics simulations

Conference Services

1. Transportation Guide

From Meilan International Airport to the Conference Venue:

a) Airport Express (机场 1 路):

Frequency: Every 30 minutes, operating from 6:30 AM to 10:00 PM.

Journey Time: Approximately 1 hour and a half.

Cost: Around 20 Yuan one way.

b) Taxi:

Journey Time: Depending on the traffic, around 40 minutes to 1 hour.

Cost: Around 50 to 90 Yuan one way.

2. Weather

Day	Temperature	Weather	Suggested wear
23 Nov	21 - 27℃	Sunny and cloudy	Short-sleeved
24 Nov	22 - 26℃	Cloudy with light rain	Short-sleeved
25 Nov	22 - 25℃	Cloudy with light rain	Short-sleeved
26 Nov	20 - 25℃	Sunny and cloudy	Short-sleeved