

International Conference on Theoretical and High Performance Computational Chemistry 2024

CONFERENCE GUIDE



19 - 22 April 2024

Wuhan, China

	Friday 19 April	Session Chair	Saturday 20 April	Session Chair	Sunday 21 April	Session Chair	Monday 22 April
Morning Session 8:30 - 12:30	—	Session 1 Chaoyuan Zhu	Opening Yasuhiro Matsunaga Yiqin Gao Xin Xu Group Photo Junichi Ono Zenghui (John) Zhang Giovanni Brandani Fei Xu	Session 5 Jing Ma	Takashi Sumikama Xiang Sun Suyong Re Xiaotian Qi Poster Session Tong Zhu Ming Lei Deping Hu Xinping Wu	Session 9 Hongxing Zhang	Jingde Bu Bo Song Qingchuan Zheng Zunnan Huang Dingguo Xu Fei Xia Xuelu Ma
Lunch 12:30 - 13:30		Buffet		Buffet		Buffet	
Afternoon Session 14:00 - 18:30	Registration 14:00 - 21:00	Session 3 Xin Xu	Hiroshi Fujisaki Fenglong Gu Bingbing Suo Wei Li (NJU) Hui Li Xuebo Chen Rongzhen Liao Jing Xie Yiyang Yang Bing Yin Weiwei Xue	Session 7 Yasuhiro Matsunaga	Osamu Miyashita Xiang Sheng Jun Ohnuki Honghui Shang Weile Jia Runfeng Jin Lihua Bie Yibo Wang Wei Li (HUNAU) Guanghui Chen Qiang Zhang Li Dang Awards & Closing	—	
Dinner 18:30 - 19:30	Buffet	Banquet		Buffet			

International Conference on Theoretical and High Performance Computational Chemistry 2024

(ICT-HPCC24)

1. Conference Information

- a) Date: 19 - 22 April 2024
- b) City: Wuhan, Hubei, China
- c) Website: <http://ict-hpcc.vlcc.cn/>
- d) Address: International Academic Exchange Center, Huazhong Agricultural University (No.1 Shizishan Street, Hongshan District, Wuhan City, Hunan Province)
(湖北省武汉市洪山区狮子山街 1 号华中农业大学国际学术交流中心)

2. Conference Room

Lecture hall, Level 1, Building 1, International Academic Exchange Center

3. Meals

e) Lunch

20/21/22 April: 12:30-14:00, Level 2, Building 1

f) Dinner/Banquet

19/20/21 April: 18:30-20:00, Level 2, Building 1

4. Poster Session

Date: 21 April 10:10 ~ 10:50

Place: Lecture hall, Level 1, Building 1

5. Contacts

Jing LI	86-10-58812172/ 86-13520969978
Baohua ZHANG	86-13581885294
Qian LIU	86-15201280496

6. Organizations

- **Chair**

- Yasuhiro Matsunaga (Saitama University, Japan)

- **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**

- Zhong Jin (Computer Network Information Center, CAS, China)
- Chaoyuan Zhu (Huazhong Agricultural University, China)
- Jun Gao (Huazhong Agricultural University, China)

- ▲ **Secretary**

- Jing Li (Computer Network Information Center, CAS, China)
- Lihua Bie (Huazhong Agricultural University, China)

7. Organizers & Sponsors

- ▲ **Organizers**

- Computer Network Information Center, Chinese Academy of Sciences (CNIC, CAS)
- Huazhong Agricultural University

- ▲ **Sponsors**

- Bureau of International Cooperation, Chinese Academy of Sciences
- Sugon

PROGRAM

Friday, 19 April

- 14:00 - 21:00** **Registration** Level 1 Lobby, Building 1
- 18:30 - 19:30** **Welcome Reception Dinner** Level 2 Multifunctional hall, Building 1

Saturday, 20 April

- 8:30 - 8:50** **Opening**
- 8:50 - 9:00** **Group Photo**

Session 1

- Session Chair** **Chaoyuan Zhu** *Huazhong Agricultural University*
- 9:00 - 9:25** **Yasuhiro Matsunaga** *Saitama University*
Integrative modeling of biomolecular dynamics from simulations and single-molecule experiments
- 9:25 - 9:50** **Yiqin Gao** *Peking University*
Recent development of a molecular simulation package
- 9:50 - 10:15** **Xin Xu** *Fudan University*
Structural Assignment of Natural Products: The SVM-M Model Based on the ¹³C NMR Chemical Shifts
- 10:15 - 10:35** **Group Photo & Break**

Session 2

- Session Chair** **Zexing Cao** *Xiamen University*
- 10:35 - 11:00** **Junichi Ono** *Waseda University*
Clarification of reaction mechanisms in biomolecules by quantum molecular dynamics simulations
- 11:00 - 11:25** **Zenghui (John) Zhang** *New York University Shanghai*
Quantum mechanical calculation of protein energies and machine learning force field
- 11:25 - 11:50** **Giovanni Brandani** *Kyoto University*
An integrative approach to the molecular modeling of genes
- 11:50 - 12:15** **Fei Xu** *Jiangnan University*
Computational Design of Collagen Nanomaterials
- 12:30 - 13:30** **Lunch** Level 2 Multifunctional hall, Building 1

Session 3

Session Chair	Xin Xu	<i>Fudan University</i>
14:00 - 14:25	Hiroshi Fujisaki	<i>Nippon Medical School</i> Weighted ensemble simulations for conformational change of biomolecules
14:25 - 14:50	Fenglong Gu	<i>South China Normal University</i> TDDFT/TDHF Methods Based on Non-Orthogonal Localized Molecular Orbitals and Its Applications
14:50 - 15:15	Bingbing Suo	<i>Northwest University</i> New approaches to accelerating self-consistent-field calculation: from heterogeneous computing to improving the SCF convergence
15:15 - 15:40	Wei Li	<i>Nanjing University</i> Low Scaling Electronic Structure Methods for Structure and Spectroscopy of Large Systems
15:40 - 16:05	Hui Li	<i>Jilin University</i> The paradigm of “theoretical model + machine learning”: Case studies of potential energy surface construction and vibrational spectra simulation
16:05 - 16:20	Break	

Session 4

Session Chair	Daiqian Xie	<i>Nanjing University</i>
16:20 - 16:55	Xuebo Chen	<i>Beijing Normal University</i> Research and development of optical functional materials based on excited state theoretical models and data
16:55 - 17:20	Rongzhen Liao	<i>Huazhong University of Science and Technology</i> Mechanistic aspects of redox reactions catalyzed by iron enzymes
17:20 - 17:45	Jing Xie	<i>Beijing Institute of Technology</i> Deciphering the Acceleration Mechanisms of Organic Reactions in Microdroplets
17:45 - 18:00	Yiyang Yang	<i>Shandong University</i> Illuminating Tandem Reactions Characterized by Temporal Separation of Catalytic Activities via DFT Calculations: A Case Study of Ni-Catalyzed Alkyne Semihydrogenation
18:00 - 18:15	Bing Yin	<i>Northwest University</i> Combined ab initio electronic structure calculation and crystal field analysis. A suitable theoretical tool for single molecule magnet

18:15 - 18:30 **Weiwei Xue** *Chongqing University*
 Computational chemistry in structure-based design of dopamine transporter allosteric inhibitors

18:30 - 20:00 **Banquet** Level 2 Multifunctional hall, Building 1

Sunday, 21 April

Session 5

Session Chair **Jing Ma** *Nanjing University*

8:30 - 8:55 **Takashi Sumikama** *Kanazawa University*
 Computational and theoretical studies in collaboration with experiments to elucidate biological phenomena

8:55 - 9:20 **Xiang Sun** *New York University Shanghai*
 Theoretical Modeling Approaches for Ultrafast Charge Transfer Dynamics in Solar Energy Conversion

9:20 - 9:45 **Suyong Re** *National Institutes of Biomedical Innovation*
 Molecular dynamics simulation of glycan cluster shielding on Lassa Virus Envelop Protein

9:45 - 10:10 **Xiaotian Qi** *Wuhan University*
 Developing new bonding models for radical coupling reactions

10:10 - 10:50 **Break & Poster Session**

Session 6

Session Chair **Qian Peng** *Nankai University*

10:50 - 11:15 **Tong Zhu** *East China Normal University*
 Automated Generation of Reaction Paths

11:15 - 11:40 **Ming Lei** *Beijing University of Chemical Technology*
 Mechanism-based Rational Catalyst Design For the Hydrogenation of C=O/C=N Double Polar Bond

11:40 - 12:05 **Deping Hu** *Beijing Normal University*
 Nonadiabatic Dynamics Simulation of the Molecular Polaritons Inside an Optical Cavity

12:05 - 12:20 **Xinping Wu** *East China University of Science and Technology*
 Level-Shifted Embedded Cluster Method and Its Applications

12:30 - 13:30 **Lunch** Level 2 Multifunctional hall, Building 1

Session 7

Session Chair	Yasuhiro Matsunaga	<i>Saitama University</i>
14:00 - 14:25	Osamu Miyashita	<i>RIKEN Center for computational Science</i>
	Integrative modeling approach combining molecular dynamics simulations and experimental data to study dynamic structures of biological molecules	
14:25 - 14:50	Xiang Sheng	<i>Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences</i>
	The Quantum Chemical Modeling in Biocatalysis	
14:50 - 15:15	Jun Ohnuki	<i>Institute for Molecular Science</i>
	Integration of AlphaFold with Molecular Dynamics to Uncover Missing Conformational States of Transporter Proteins	
15:15 - 15:40	Honghui Shang	<i>University of Science and Technology of China</i>
	Large-scale quantum emulating simulations of biomolecules: A pilot exploration of parallel quantum computing	
15:40 - 16:05	Weile Jia	<i>Institute of Computing Technology, Chinese Academy of Sciences</i>
	Fast rt-TDDFT Calculations with Parallel Transport Gauge and Hybrid Functional	
16:05 - 16:20	Break	

Session 8

Session Chair	Jun Gao	<i>Huazhong Agricultural University</i>
16:20 - 16:35	Runfeng Jin	<i>Computer Network Information Center, Chinese Academy of Sciences</i>
	PASCI: A Scalable Framework for Massively Heterogeneous Parallel Calculation of Dynamical Electron Correlation	
16:35 - 16:50	Lihua Bie	<i>Huazhong Agricultural University</i>
	Porting and optimization of the exchange-correlation functional library Libxc on the heterogeneous platform	
16:50 - 17:05	Yibo Wang	<i>Changchun Institute of Applied Chemistry, Chinese Academy of Sciences</i>
	Stereoselective recognition of morphine enantiomers by μ -opioid receptor	
17:05 - 17:20	Wei Li	<i>Hunan Agricultural University</i>
	Nonadiabatic Dynamics in Metal Halide Perovskites	

- 17:20 - 17:35** **Guanghai Chen** *Shantou University*
Data-mining based assembly of promising metal-organic frameworks on Xe/Kr separation
- 17:35 - 17:50** **Qiang Zhang** *Inner Mongolia Minzu University*
Energy Relaxation and Multi-scale Molecular Dynamics at Hydration Interface
- 17:50 - 18:05** **Li Dang** *Shantou University*
Room Temperature Phosphorescence Polymer Doped with Fluorescent Molecules by Electronic Structure Study
- 18:05 - 18:30** **Awards & Closing**
- 18:30 - 19:30** **Dinner** Level 2 Multifunctional hall, Building 1

Monday, 22 April

Quantum Biology and Bioinformatics Forum (Chinese)

Session 9

Session Chair	Hongxing Zhang 张红星	<i>Jilin University</i>
8:30 - 8:55	Jingde Bu 卜景德	
	Computational chemistry practices on deep compute heterogeneous platform	
8:55 - 9:20	Bo Song 宋波	<i>University of Shanghai for Science and Technology</i>
	ATP-photons and Quantum Neuron	
9:20 - 9:45	Qingchuan Zheng 郑清川	<i>Jilin University</i>
	细胞色素 P ₄₅₀ 3A ₄ 介导的咪达唑仑代谢机制	
9:45 - 10:10	Zunnan Huang 黄遵楠	<i>Guangdong Medical University</i>
	大数据挖掘和精准药物设计	
10:10 - 10:30	Break	

Session 10

Session Chair	Dongju Zhang 张冬菊	<i>Shandong University</i>
10:30 - 10:55	Dingguo Xu 徐定国	<i>Sichuan University</i>
	羟基磷灰石的第一性原理、分子动力学及机器学习研究	
10:55 - 11:20	Fei Xia 夏飞	<i>East China Normal University</i>
	微管全原子与粗粒化杂化模型的最新发展	
11:20 - 11:55	Xuelu Ma 马雪璐	<i>China University of Mining and Technology, Beijing</i>
	Theoretical studies on the mechanism of dinitrogen fixation catalyzed by trinuclear transition metal complexes	
12:00 - 13:00	Lunch	Level 2 Multifunctional hall, Building 1

POSTER SESSION

Sunday, 21 April 10:10 - 10:50, Level 1, Building 1

- P1** **Theoretical study on the complexes formed by CF₃I with ethyne, ethene, and ethane**
Huimin Zhang, Minghui Yang*
- P2** **Unified Model to Predict gRNA Efficiency across Diverse Cell Lines and CRISPR-Cas9 Systems**
Zhicheng Zhong, Qian Wang
- P3** **Theoretical study on the complexes formed by CF₃I with CO and N₂**
Mingjuan Yang, Minghui Yang*
- P4** **Predicting the Rate Constants of Hydrogen Abstraction Reactions between OH/HO₂ and Alkanes by Machine Learning Model**
Min Xia, Yu Zhang, Hongwei Song, Ya Jia, Minghui Yang
- P5** **Construction of a Globally Accurate Potential Energy Surface for the F+H₂O₂ Reaction**
Yizhuo Chen, Hongwei Song, Chuanxi Duan
- P6** **Mechanistic studies of photoredox/nickel catalyzed ligand-controlled regioversed aryl-aminoalkylation of alkenes**
Yixin Luo
- P7** **Accurate prediction of bulk heterojunction morphology by acceptor material monomers**
Yizhou Xu, Guangyan Sun*
- P8** **Theoretical study of photocatalytic properties of porous frameworks**
Zi-jian Zhou, Xin-Ping Wu*
- P9** **Charged Histidine Residues Govern the pH-dependent Assembling of Toll-like Receptor 3 on dsRNA**
Penghui Li
- P10** **Development of topology-based descriptors for adsorptions and reactions on catalyst surfaces**
Zhao-Bin Ding
- P11** **Fail-Safe Quantum Chemical Calculations with Improved Machine-Learning Models**
Yuan, Kai; Zhou, Shuai; Li, Ning; Li, Tianyan; Ding, Bowen*; Guo, Danhuai*; Ma, Yingjin*

- P12** **Development of the extended coarse-grained (XCG) model: accurate, easy-to-construct and excellent inter-system transferability**
Yuwei Zhang, Xin Xu*
- P13** **Theoretical study of weak intramolecular and intermolecular interactions modulating energy/charge transfer behavior in organic solar cells**
Rui-Cheng Qin, Ming-Yang Li*, Guang-Yan Sun*
- P14** **Development of milestoning and committor functions in milestoning**
Ru Wang
- P15** **Reaction Coordinate Identification and Free Energy Decomposition Analysis from Transition Path Ensemble**
Wenjin Li
- P16** **Research on Fragment-based Methods and Load Balancing in Qbio Package**
Jian-Ping Guo
- P17** **Energy transfer pathways of red algae Porphyridium purpureum phycobilisome (PBS) - PSII - PSI - LHC megacomplex based on exciton model**
Meng-Ying Tong
- P18** **Ion coherence: A physical derivation of high-flux ion transport in biological channel**
Yue Wang
- P19** **Migration and optimization of Density Functional Theory mpec + cosx library**
Kai-Yu He
- P20** **Research on the Ion Transmission Mechanism of Piezo1**
Quan Wen
- P21** **Research on multi-granularity sequence alignment parallel algorithm based on the Sunway platform**
Ao Shen
- P22** **A potent eEF2K inhibitor with in vivo anti-tumor metastatic activity**
Dengjie Yan, Xiaoyu Guo, Nan Wu, Kevin N. Dalby, Qiantao Wang*

CONFERENCE SERVICES

1. Transportation Guide

Note: If taking a taxi, you can drive in through the **west gate** of the university and directly take off at the conference venue. If you go to the other gates of the university, you can only take off at the gate and walk in.

If travelling by public transport, you can come in through the **west gate** of the university and take the **on-campus bus Route 1** (校园巴士 1 号线) directly to the conference venue. If you come in through the other gates, you can only walk to the conference venue, it takes around 10 minutes.

The **bus stops** near the university:

- Bus 571/576/908/591/905: Huazhong Agricultural University Station, South Luoshi Road (珞狮南路华中农大站) - near **west gate**

- Bus 570: North Station of Huazhong Agricultural University, South Lake Avenue Station (南湖大道华中农大北站) - near north gate

1) From **WUHAN TIANHE International Airport:**

a) **Taxi:**

Journey Time: Approximately 60 minutes.

Cost: RMB 100-150 one way, depending on the traffic.

b) **Subway + Bus:**

Journey Time: Approximately 120 minutes.

Cost: Around RMB 11 one way.

How to take it:

1. Take the Subway line 2 at Tianhe Airport Station (天河机场站) and transfer to Buddha Ridge (佛祖岭) for 22 stops, then take off at Baotong Temple Station (宝通寺站) and exit the subway at Exit A.

2. Take 2-minute walk to the bus stop, take Bus 576 from Wuluo Road Subway Station (武珞路地铁站) for 11 stops to take off at Huazhong Agricultural University Station, South Luoshi Road (珞狮南路华中农大站).

3. Take the on-campus bus route 1 (校园巴士 1 号线) and take off at International Academic Exchange Centre (国际学术交流中心站).

c) High-speed Train + Bus (be sure to check flight arrival times and train times):

Journey Time: Approximately 90-100 minutes.

Cost: Around RMB 16 one way.

How to take it:

1. Take the high-speed train at the airport at Tianhe Airport Station (天河机场站) for 2 stops and take off at Wuchang Railway Station (武昌站).

2. Take bus 571 (from Zhongshan Road Wuchang Railway Station 中山路武昌火车站, 16 stops) or bus 908 (from Wuchang Railway Station Bus Stop 武昌火车站公交场站, 13 stops) and take off at Huazhong Agricultural University Station, South Luoshi Road (珞狮南路华中农大站).

3. Take the on-campus bus route 1 (校园巴士 1 号线) and take off at International Academic Exchange Centre (国际学术交流中心站).

2) From WUCHANG railway station (武昌站):

a) Taxi:

Journey Time: Approximately 30 minutes.

Cost: Around RMB 30 one way, depending on the traffic.

b) Public transport:

Journey Time: Approximately 45-50 minutes.

Cost: RMB 3 one way.

How to take it:

1. Take bus 571 (from Zhongshan Road Wuchang Railway Station 中山路武昌火车站, 16 stops) or bus 908 (from Wuchang Railway Station Bus Stop 武昌火车站公交场站, 13

stops) and take off at Huazhong Agricultural University Station, South Luoshi Road (珞狮南路华中农大站).

2. Take the on-campus bus route 1 (校园巴士 1 号线) and take off at International Academic Exchange Centre (国际学术交流中心站).

3) From **WUHAN railway station (武汉站):**

a) Taxi:

Journey Time: Approximately 35 minutes.

Cost: Around RMB 60 one way, depending on the traffic.

b) Public transport:

Journey Time: Approximately 75-80 minutes.

Cost: RMB 9 one way.

How to take it:

1. Take the Subway line 4 at Wuhan Railway Station (武汉火车站) board for Bolin (柏林) for 7 stops, then take off at Yuejiazui Station (岳家嘴站).

2. Transfer to Subway line 8 board for Junyun Village (军运村) for 9 stops, and take off at Wenzhi Street station(文治街站), exit the subway at Exit B.

3. Take 2-minute walk to the bus stop, take Bus 591/576/905/W567 from Luoshi Road Wenzhi Street Station (珞狮路文治街站) for 5 stops to take off at Huazhong Agricultural University Station, South Luoshi Road (珞狮南路华中农大站).

4. Take the on-campus bus route 1 (校园巴士 1 号线) and take off at International Academic Exchange Centre (国际学术交流中心站).

4) From **HANKOU railway station (汉口站):**

a) Taxi:

Journey Time: Approximately 40 minutes.

Cost: Around RMB 80 one way, depending on the traffic.

b) Public transport:

Journey Time: Approximately 80 minutes.

Cost: RMB 8 one way.

How to take it:

1. Take the Subway line 2 at Hankou railway station (汉口火车站) board for Buddha Ridge (佛祖岭) for 12 stops, then take off at Baotong Temple Station (宝通寺站) and exit the subway at Exit A.
2. Take 2-minute walk to the bus stop, take Bus 576 from Wuluo Road Subway Station (武珞路地铁站) for 11 stops to take off at Huazhong Agricultural University Station, South Luoshi Road (珞狮南路华中农大站).
3. Take the on-campus bus route 1 (校园巴士 1 号线) and take off at International Academic Exchange Centre (国际学术交流中心站).

2. Weather

Day	Temperature	Weather	Suggested wear
19 April, Friday	14 - 22 °C	Cloudy	Windbreaker or thin jacket
20 April, Saturday	13 - 22 °C	Cloudy	Windbreaker or thin jacket
21 April, Sunday	14 - 24 °C	Cloudy	Windbreaker or thin jacket
22 April, Monday	15 - 24 °C	Cloudy	Windbreaker or thin jacket

3. Conference Site Map

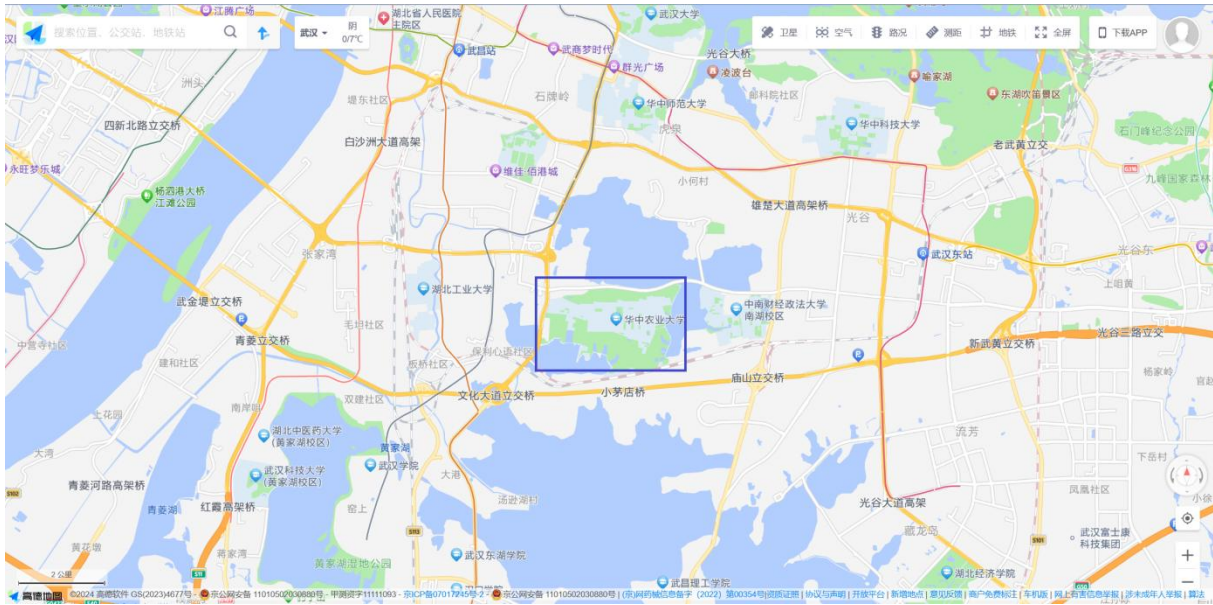


West Gate of Huazhong Agricultural University



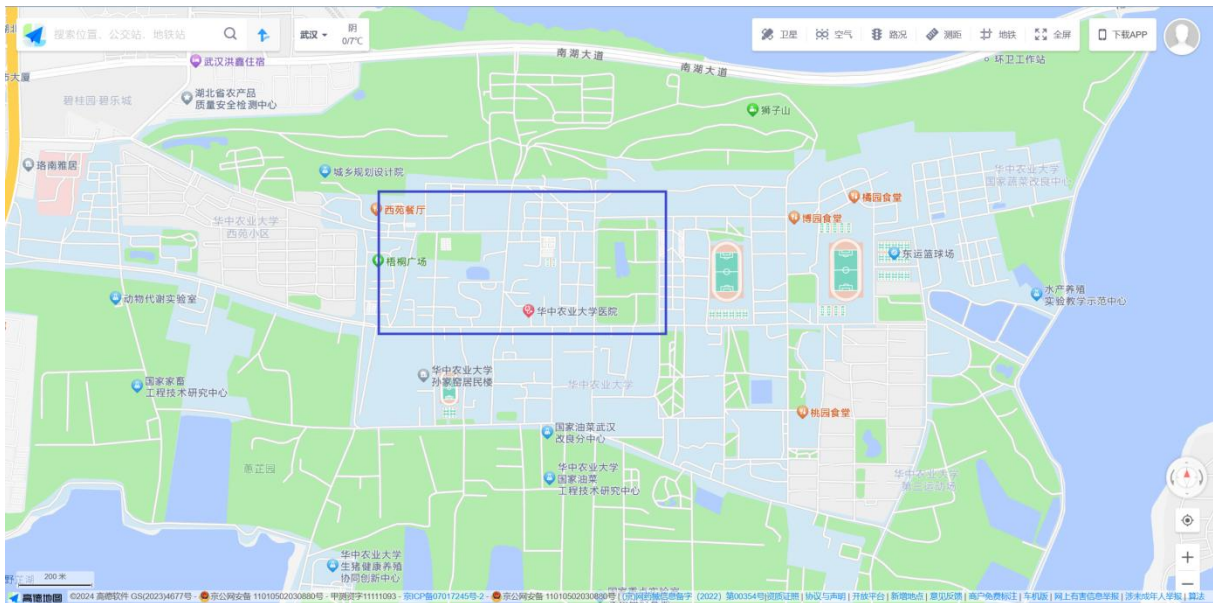
International Academic Exchange Center, Huazhong Agricultural University

Campus Map:



Where Huazhong Agricultural University located

Zoom in ↓



Around where the International Academic Exchange Center, Huazhong Agricultural University located

