ISTCP 2024

11th Triennial Congress of the International Society for Theoretical Chemical Physics

Conference Proceeding

October 13-18, 2024, Qingdao, China

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ISTCP 2024

Words of Welcome

On behalf of the local organizing committee, it is a great pleasure for me to wish you all welcome to the 11th triennial congress of the International Society of Theoretical Chemical Physics, ISTCP-2024, which will provide a unique opportunity to be updated on the latest scientific development and to develop new scientific ideas.

The program of the conference follows the successful recipe of earlier conferences, and will consist of plenary speakers and invited talks in a series of parallel sessions. In addition, there will be poster presentations that are open to contributions from all participants. The venue, compact and situated in a central location, in combination with the invigorating sea breeze and the crisp Tsingtao beer on offer, should help create an atmosphere that stimulates the exchange of scientific ideas.

For many, the conference will be the first opportunity to visit Qingdao, and I encourage you use the opportunity to also explore North China either prior to or after conference. We will organize several tour options for the free afternoon of the conference, as well as the option to take a cable car (or hike) to the top of a Laoshan mountain overlooking the entire Qingdao city.

I look forward to welcoming you to the 11th congress of the ISTCP 2024.

Wenjian Liu, Chair of ISTCP-2024

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PROGRAM AT A GLANCE

Sunday, 13 October 2024

Time	Huanghai Hotel Lobby (黄海饭店大堂)
08:30-16:00	Registration

Time	Room 1 & 2, 1st floor (二楼会议中心)	
16:00-16:40	Opening Ceremony	Chair: Wenjian Liu
16:40-18:10	Plenary Lectures	
	David Clary	Chair: William Miller
	Hiroshi Nakatsuji	Chair: Wenjian Liu

Time	Dining Hall on the ground and first floor
18:30-21:00	Welcome Reception

Monday, 14 October 2024

Time	Room 1 & 2, 1st floor (二楼会议中心)					
08:30-10:00	Plenary Lectures					
	Martin Head-Gordon				Chair: DanielCrawford	
	Odile Eisenstein				Chair: Zhigang Shuai	
10:00-10:30	Coffee Break					
	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
10:30-12:00	ENDS Section 1 Chair: Wolfgan Domcke William Miller Jian Liu	DFT Section 1 Chair: Weitao Yang Lucia Reining Jianwei Sun Yang Yang	SPECT Section 1 Chair: Yi Luo Trond Saue Hui Li Wanzhen Liang	O(N) Section 1 Chair: Edward Valeev Masato Kobayashi Kaori Fukuzawa	SOFT Section 1 Chair: Daniel Crawford Giuseppe Barca Yingjin Ma Wei Hu	MEM Section 1 Chair: Yuxiang Bu Shubin Liu Dongxia Zhao Thijs Stuyver
12:00-13:30	Lunch Break, Sponsor Lecture by ByteDance in Room 4					
13:30-15:30	ENDS Section 2 Chair: William Miller Nancy Makri Jiushu Shao Michael Thoss Zhonghan Hu	MLDD Section 1 Chair: Jonathan Hirst Steven Lopez Sungnam Park Alexei Kananenka Weiluo Ren	CAT Section 1 Chair: Jun Li Sergey Kozlov Weixue Li Núria López Alexander Bagger	EMBED Section 1 Chair: Tianyu Zhu Troy van Voorhis Emmanuel Fromager Hong Jiang Marco Govoni	SPECT Section 2 Chair: Leticia Gonzalez Yi Luo Héléne Bolvin Mathieu Linares Qiang Shi	BIO Section 1 Chair: Nadia Elghobashi-Meinhardt Qiang Cui Peter Kekenes-Huskey Sichun Yang
15:30-16:00	Coffee Break					
16:00-18:00	ENDS Section 3 Chair: Jian Liu Benjamin Levine Chaoyuan Zhu Zhenggang Lan Amber Jain	WFT Section 1 Chair: Piotr Piecuch Shuhua Li Debashree Ghosh Haibo Ma	CAT Section 2 Chair: Xiaojing Liu Karoliina Honkala Evgeny Pidko Hai Xiao Jia Zhang	MATER Section 1 Chair: De-en Jiang Xiaocheng Zeng Jinlan Wang Sergey Levchenko Zhongyuan Lu	SPECT Section 3 Chair: Robert Berger Leticia Gonzalez Bing Gu Elke Fasshauer Attila Császár	QC4QC Section 1 Chair: Zhenyu Li Joonho Lee Zhendong Li Junxu Li
19:30-21:30	Hallway on the first floor (二楼会议中心走廊)					
	Poster Session 1					

Tuesday, 15 October 2024

Time	Room 1 & 2, 1st floor (二楼会议中心)					
08:30-10:00	Plenary Lectures					
	Weitao Yang				Chair: Xin Xu	
	Anna Krylov				Chair: Peter Surjan	
10:00-10:30	Coffee Break					
	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
10:30-12:00	WFT Section 2 Chair: Haibo Ma Claudia Filippi Alex Thom Janus Juul Eriksen	DFT Section 2 Chair: James Patrick Lewis Xin Xu Pina Romaniello Xiao Zheng	MLDD Section 2 Chair:Arif Ullah Pavlo O. Dral Jing Ma Zhou Lin	BIO Section 2 Chair: Qiang Cui Jin Yong Lee Munir Salomao Skaf Yi Wang	Relativity Section 1 Chair: Xiaosong Li Anastasia Borschevsky Edit Mátyus Agustín Aucar	MEM Section 2 Chair: Shubin Liu Yuxiang Bu Peifeng Su
12:00-13:30	Lunch Break, Sponsor Lecture by MattVerse in Room 4					
13:30-15:30	ENDS Section 4 Chair: Michael Thoss Donghui Zhang Tucker Carrington Françoise Remacle Oriol Vendrell	WFT Section 3 Chair: Jiří Pittner Katarzyna Pernal Jae Woo Park Ágnes Szabados Yang Guo	CAT Section 3 Chair: Weixue Li Anastassia Alexandrova Jun Li Nicola Gaston Natalie Gelfand	MATER Section 2 Chair: Linjun Wang David Beljonne Zhigang Shuai Daniel Escudero Aijun Du	SPECT Section 4 Chair: Attila Császár Trygve Helgaker Sonia Coriani Daniel Crawford Michal Repisky	MLDD Section 3 Chair: Milica Todorović Jonathan Hirst Jacqueline Cole Guido von Rudorff Miao Liu
15:30-16:00	Coffee Break					
16:00-18:00	ENDS Section 5 Chair: Tucker Carrington Chun-Wei Pao Jianshu Cao Seogjoo Jang Yi Zhao	DFT Section 3 Chair: Emmanuel Fromager Andrew Teale Igor Ying Zhang Neil Qiang Su James Patrick Lewis	BIO Section 3 Chair: Steven Schwartz Jin Wang Nadia Elghobashi-Meinhardt Wei Zhuang Yiqin Gao	MATER Section 3 Chair: Aijun Du Wenjie Dou Linjun Wang Elena Besley Xiaojun Wu	EMBED Section 2 Chair: Troy van Voorhis Tianyu Zhu William Glover	SOFT Section 2 Chair: Edward Valeev Hujun Qian Steven Kirk Zikuan Wang Jingxiang Zou
19:30-21:30	Hallway on the first floor (二楼会议中心走廊)					
	Poster Session 2					

Wednesday, 16 October 2024

Time	Room 1 & 2, 1st floor (二楼会议中心)					
08:30-10:00	Plenary Lectures					
	Yundong Wu				Chair: Yiqin Gao	
	Laura Gagliardi				Chair: Trygve Helgaker	
10:00-10:30	Coffee Break					
	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
10:30-12:00	CAT Section 4 Chair: Anastassia Alexandrova Jun Cheng Christopher Stein Qian Peng	MLDD Section 4 Chair: Pavlo O. Dral Lipeng Chen Jin Wen Arif Ullah	MATER Section 4 Chair: Weiqiao Deng Momoji Kubo De-en Jiang Karsten Reuter	O(N) Section 2 Chair: Haibo Ma Edward Valeev John Herbert	EMBED Section 3 Chair: William Glover Christoph Jacob Michele Pavanello Dingshun Lv	QC4QC Section 2 Chair: Zhendong Li Rahul Maitra Zhenyu Li Yuchen Wang
12:00-13:30	Lunch Break					
13:30-18:30	Excursions					
18:30-21:00	Room 1 & 2, 1st floor (二楼会议中心)					
	Conference Dinner					

Thursday, 17 October 2024

Time	Room 1 & 2, 1st floor (二楼会议中心)					
08:30-10:00	Plenary Lectures					
	Eberhard K.U. Gross				Chair: Edward Valeev	
	Jiali Gao				Chair: Shuhua Li	
10:00-10:30	Coffee Break					
	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
10:30-12:00	ENDS Section 6 Chair: Mark Tuckerman Zlatko Bačić Yijing Yan Jiří Vaníček	CAT Section 5 Chair: Sergey Kozlov Luigi Cavallo Ming Lei Andrew Rappe	DFT Section 4 Chair: Ilaria Ciofini Wei Wu Chen Li Timothy Gould	O(N) Section 3 Chair: Shuhua Li Michael Dolg Yuriko Aoki Ganglong Cui	SPECT Section 5 Chair: Trygve Helgaker Robert Berger Christoph van Wüllen	SOFT Section 3 Chair: Wei Hu Qiming Sun Jun Zhang Youliang Zhu
12:00-13:30	Lunch Break, Sponsor Lecture by AI-chem in Room 4					
13:30-15:30	ENDS Section 7 Chair: Zhonghan Hu Mark Tuckerman Maxim Gelin Samantha Jenkins Michał Tomza	WFT Section 4 Chair: Pierre-François Loos Piotr Piecuch Feiwu Chen Katharina Boguslawski Jiří Pittner	CAT Section 6 Chair: Jun Cheng Zhipan Liu Mikhail V. Polynski Jilai Li Xiaojing Liu	BIO Section 4 Chair:Yaoqi Zhou Steven Schwartz Barak Hirshberg Jing Huang Wenning Wang	MATER Section 5 Chair: Yuchen Ma Weiqiao Deng Krzysztof Szalewicz Dongwook Kim	MLDD Section 5 Chair: Jacqueline Cole Guanhua Chen Jun Jiang Milica Todorović
15:30-16:00	Coffee Break					
16:00-18:00	DFT Section 5 Chair: Igor Ying Zhang Ilaria Ciofini Cheol Ho Choi Eduard Matito Bruno Senjean	WFT Section 5 Chair: Katarzyna Pernal Mark R. Hoffmann Mihály Kállay Thomas Jagau Ke Liao	Relativity Section 2 Chair: Eugene DePrince André Severo Pereira Gomes Jing Su Minori Abe	BIO Section 5 Chair: Wei Zhuang Yaoqi Zhou Pietro Faccioli Hao Wang Jun Gao	QC4QC Section 3 Chair: Junxu Li Kosuke Mitarai Xiao Yuan Zixuan Hu	
19:30-21:30	Hallway on the first floor (二楼会议中心走廊)					
	Poster Session 3					

Friday, 18 October 2024

Time	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
08:30-10:00	WFT Section 6 Chair: Yang Guo Pierre-François Loos Andreas Grüneis Zhenhua Chen	DFT Section 6 Chair: Xin Xu Juan Felipe Huan Lew-Yee Fenglong Gu Jan M. L. Martin	MLDD Section 6 Chair: Jin Wen Dongqing Wei Hanshi Hu Lin Shen	EMBED Section 4 Chair: Hong Jiang Matthew Hermes Tomasz A. Wesolowski Lyudmila Slipchenko	Relativity Section 3 Chair: André Severo Pereira Gomes Eugene DePrince Xiaoyan Cao Xiaosong Li	MEM Section 3 Chair: Odile Eisenstein Krzysztof Szalewicz Piotr Piecuch Hui Li
10:00-10:30	Coffee Break					
10:30-11:15	Room 1 & 2, 1st floor (二楼会议中心) Plenary Lecture Debashis Mukherjee				Chair: Mark R Hoffmann	
11:15-12:00	Closing Ceremony				Chair Wenjian Liu	

SCIENTIFIC PROGRAM

PROGRAM - SUNDAY, 13 October 2024

Time	Huanghai Hotel Lobby (黄海饭店大堂)
08:30-16:00	Registration

Time	Room 1 & 2, 1st floor (二楼会议中心)	
16:00-16:40	Opening Ceremony	Chair: Wenjian Liu
16:40-17:25	Plenary Lecture *David Clary* Schrödinger, Born and Kohn: Pioneers in theoretical chemical physics	Chair: William Miller
17:25-18:10	Plenary Lecture *Hiroshi Nakatsuji* Theoretical chemistry based on the exact solutions of the scaled Schrödinger equation	Chair: Wenjian Liu

Time	Dining Hall on the ground and first floor
18:30-21:00	Welcome Reception

PROGRAM - MONDAY, 14 October 2024

Time	Room 1 & 2, 1st floor (二楼会议中心)					
08:30-09:15	Plenary Lecture *Martin Head-Gordon* MP2 made better and faster? Recent developments in regularization and local correlation				Chair: Daniel Crawford	
09:15-10:00	Plenary Lecture *Odile Eisenstein* Nucleophilic addition: Input from computations from the Felkin-Anh rule to the Grignard reaction				Chair: Zhigang Shuai	
10:00-10:30	Coffee Break					
	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
10:30-12:00	ENDS Section 1 Chair: Wolfgang Domcke	DFT Section 1 Chair: Weitao Yang	SPECT Section 1 Chair: Yi Luo	O(N) Section 1 Chair: Edward Valeev	SOFT Section 1 Chair: Daniel Crawford	MEM Section 1 Chair: Yuxiang Bu
10:30	*William Miller* Classical molecular dynamics simulations of electronically non-adiabatic processes	*Lucia Reining* Design principles for functionals based on systematic expansions	*Trond Saue* Beyond the Dailey-Townes model: Chemical information from the electric field gradient	*Masato Kobayashi* Recent advances in divide-and-conquer quantum chemistry: toward large scale and beyond	*Giuseppe Barca* Fast quantum chemistry on multi-GPU architectures: Achievements and future directions	*Shubin Liu* Harnessing chemical understanding with wave function theory, density functional theory, machine learning, and quantum computers
11:00	*Jian Liu* Nonadiabatic field: A conceptually new approach for nonadiabatic dynamics	*Jianwei Sun* Unveiling the origins of DFT errors in open-shell d- and f-electron compounds: An analysis of scan's performance in addressing self-interaction error and strong correlation, with enhanced SIE reduction within semilocal approximations	*Hui Li* Developing local quantum vibration embedding framework for multi-dimensional vibrational spectra	*Kaori Fukuzawa* Fragment molecular orbital calculations for biomolecules	*Yingjin Ma* "Chemical reactions" between HPC/AI and RGs	*Dongxia Zhao* Frontier electron density to characterize the molecular interaction and reactivity
11:30		*Yang Yang* Constrained nuclear-electronic orbital (CNEO) framework: Describing hydrogen-related chemistry with energy surfaces incorporating nuclear quantum effects	*Wanzhen Liang* The behaviors of molecules in strong coupling regimes		*Wei Hu* Discontinuous Galerkin Hartree-Fock calculations for predicting accurate electronic structures of mesoscopic-scale metal-semiconductor junctions with millions of atoms	*Thijs Stuyver* Efficiently learning activation energies with ml models augmented with valence bond reactivity theory derived descriptors
12:00-13:30	Lunch Break					
12:50-13:20	Sponsor Lecture: Room 4, *Xiaojie Wu (ByteDance),* Advanced scientific computation on cloud: Exploring the future of chemistry					

PROGRAM- MONDAY, 14 October 2024

Time	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
13:30-15:30	ENDS Section 2 Chair: William Miller	MLDD Section 1 Chair: Jonathan Hirst	CAT Section 1 Chair: Jun Li	EMBED Section 1 Chair: Tianyu Zhu	SPECT Section 2 Chair: Leticia Gonzalez	BIO Section 1 Chair: Nadia Elghobashi-Meinhardt
13:30	*Nancy Makri* Small matrix path integral methods for quantum dynamics	*Steven Lopez* Machine-learning-accelerated photodynamics simulations in complex environments towards new materials and medicines	*Sergey Kozlov* Role of metal-oxide interfaces in catalysis	*Troy van Voorhis* Bootstrap embedding	*Yi Luo* Molecular response under a highly confined electromagnetic field	*Qiang Cui* Analysis of allostery in a transcription factor using molecular simulations and machine learning
14:00	*Jiushu Shao* Quantum evolution represented by Brownian motion: Theory and applications	*Sungnam Park* Deep learning model for predicting optical properties of organic molecules in solutions	*Weixue Li* Heterogenous catalysis by interpretable machine learning	*Emmanuel Fromager* Density matrix embedding theory: A density (matrix) functional perspective	*Héléne Bolvin* Modeling paramagnetic NMR	*Peter Kekenes-Huskey* Characterization of intrinsic disorder in actin-binding LIM protein 1
14:30	*Michael Thoss* Simulation of quantum dynamics and transport using the hierarchical equations of motion method	*Alexei Kananenka* Machine-learning for quantum dissipative dynamics	*Núria López* Simulations in electrocatalysis	*Hong Jiang* Orthogonal and non-orthogonal local orbitals based quantum embedding approach to strongly correlated systems	*Mathieu Linares* VeloxChem: Science and education-enabling platform for quantum molecular modeling	*Sichun Yang* Integrative biophysics of ERalpha allosteric interactions and disruption
15:00	*Zhonghan Hu* On the stability of path integral molecular dynamics simulations	*Weiluo Ren* Recent Progress in Neural Network-based Quantum Monte Carlo	*Alexander Bagger* Data-driven symbiosis between computations & experiments for electrochemical reactions	*Marco Govoni* Exploration of the optical properties of point defects in semiconductors and insulators using time-dependent density functional theory and quantum embedding methods	*Qiang Shi* Chemical dynamics from the hierarchical equations of motion method: Methodology developments and applications	
15:30-16:00	Coffee Break					

PROGRAM - MONDAY, 14 October 2024

Time	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
16:00-18:00	ENDS Section 3 Chair: Jian Liu	WFT Section 1 Chair: Piotr Piecuch	CAT Section 2 Chair: Xiaojing Liu	MATER Section 1 Chair: De-en Jiang	SPECT Section 3 Chair: Robert Berger	QC4QC Section 1 Chair: Zhenyu Li
16:00	*Benjamin Levine* Ultrafast dynamics on many electronic states	*Shuhua Li* Block-correlated coupled cluster methods for strongly correlated systems	*Karoliina Honkala* Modeling electrocatalytic interfaces via advanced DFT calculations	*Xiaocheng Zeng* Computer-aided nanoscience research: Nanoice, superhydrophobicity, and topological wetting state	*Leticia Gonzalez* Disentangling spectroscopic signals with trajectory surface-hopping methods based on vibronic coupling methods	*Joonho Lee* Examining the prospects of computational quantum advantage using QC-QMC
16:30	*Chaoyuan Zhu* Global switching trajectory surface hopping molecular dynamics simulation with TDDFT potential energy surfaces	*Debashree Ghosh* Quantum chemistry methods to study strongly correlated systems – from variational to machine learning approaches	*Evgeny Pidko* Condition-dependent energy landscape of catalytic paths for activity and stability control	*Jinlan Wang* Machine learning material design and synthesis for small datasets	*Bing Gu* Exact ab initio conical intersection dynamics	*Zhendong Li* Searching for less entangled orbitals
17:00	*Zhenggang Lan* Nonadiabatic dynamics, time-resolved pump-probe spectra and machine learnings	*Haibo Ma* New quantum chemical approaches based on renormalized modes/states for large strongly correlated systems	*Hai Xiao* Potential dependence in oxygen evolution reaction	*Sergey Levchenko* Deriving catalyst design strategies from computational data using artificial intelligence	*Elke Fasshauer* Electronic decay process spectra including nuclear degrees of freedom	*Junxu Li* Toward perturbation theory methods on quantum computers
17:30	*Amber Jain* Can classical simulations sense conical intersections?		*Jia Zhang* Density functional theory studies for CO_2 conversion to value-added chemicals	*Zhongyuan Lu* Approaching larger spatial and temporal scales in polymer simulations	*Attila Császár* MARVEL, SNAPS, and hubs	
19:30-21:30	Hallway on the first floor (二楼会议中心走廊)					
	Poster Session 1					

PROGRAM - TUESDAY, 15 October 2024

Time	Room 1 & 2, 1st floor (二楼会议中心)					
08:30-09:15	Plenary Lecture *Weitao Yang* ΔSCF excited-state approach: Theoretical foundation, linear conditions for fractional charges, and physical meaning of orbital energies				Chair: Xin Xu	
09:15-10:00	Plenary Lecture *Anna Krylov* Quantum chemistry of core-level states				Chair: Peter Surjan	
10:00-10:30	Coffee Break					
	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
10:30-12:00	WFT Section 2 Chair: Haibo Ma	DFT Section 2 Chair: James Patrick Lewis	MLDD Section 2 Chair:Arif Ullah	BIO Section 2 Chair: Qiang Cui	Relativity Section 1 Chair: Xiaosong Li	MEM Section 2 Chair: Shubin Liu
10:30	*Claudia Filippi* Beyond energy: Expanding quantum Monte Carlo with derivatives	*Xin Xu* Doubly hybrid functionals: From molecules to extended materials	*Pavlo O. Dral* Universal and updatable artificial intelligence-enhanced quantum chemical foundational models	*Jin Yong Lee* Identification and isomerization of histidine tautomers in amyloid beta peptides	*Anastasia Borschevsky* Relativistic couple cluster investigations of atomic properties of the heavies elements	*Yuxiang Bu* Dynamics chemistry for the excited systems: A combined ab initio molecular dynamics and machine learning simulation strategy
11:00	*Alex Thom* Stochastic approaches to quantum chemistry	*Pina Romaniello* Optical Spectra of periodic systems from ab-initio theories	*Jing Ma* Deep learning of stability of ligand-protected gold nanoclusters	*Munir Salomao Skaf* MassCCS: Collision-cross section calculations for macromolecular assemblies	*Edit Mátyus* Bound-state relativistic quantum electrodynamics: a perspective for precision physics with atoms and molecules	*Peifeng Su* Energy decomposition analysis method for qualitative and quantitative interpretations
11:30	*Janus Juul Eriksen* Exploiting non-Abelian point-group symmetry to estimate the exact ground-state correlation energy of benzene in a polarized split-valence triple-zeta basis set	*Xiao Zheng* Developing machine-learning-corrected density functionals free from error cancellation	*Zhou Lin* Machine learned electronic structures and optical properties for organic semiconductors	*Yi Wang* Exploring plant enzyme conformations and dynamics via MD simulations	*Agustín Aucar* Role of spin-orbit effects in the relationship between NMR shielding and nuclear spin-rotation tensors	
12:00-13:30	Lunch Break					
12:50-13:20	Sponsor Lecture: Room 4, *Shuguang Chen (MattVerse),* MattVerse: Battery Design Automation (BDA) for new energy industry					

PROGRAM - TUESDAY, 15 October 2024

Time	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
13:30-15:30	ENDS Section 4 Chair: Michael Thoss	WFT Section 3 Chair: Jiří Pittner	CAT Section 3 Chair: Weixue Li	MATER Section 2 Chair: Linjun Wang	SPECT Section 4 Chair: Attila Császár	MLDD Section 3 Chair: Milica Todorović
13:30	*Donghui Zhang* Towards a quantitatively accurate universal potential for water	*Katarzyna Pernal* Basis set error-corrected multireference random phase approximations for the correlation energy	*Anastassia Alexandrova* Interfacial fluxionality in enectrocatalysis: In and out of equilibrium	*David Beljonne* Transient delocalization in conjugated organic materials	*Trygve Helgaker* A variational reformulation of molecular properties in electronic-structure theory	*Jonathan Hirst* AI4Green: An open source ELN for green and sustainable chemistry
14:00	*Tucker Carrington* An MCTDH collocation method with more points than basis functions: Obviating integrals	*Jae Woo Park* Multireference perturbation methods for exploring potential energy surfaces	*Jun Li* Atomically precise heterogeneous catalysis with graphdiyne-supported metal clusters	*Zhigang Shuai* A unified picture for carrier transport in organic semiconductors	*Sonia Coriani* In silico spectroscopy on classic and hybrid quantum computers	*Jacqueline Cole* Data-driven materials science for energy-sustainable applications
14:30	*Françoise Remacle* Electronic coherences built by an attopulse control electron-nuclei entanglement and the forces on the nuclei	*Ágnes Szabados* Perturbation-adapted PT (PAPT): Analysis and extension to the multi-reference level	*Nicola Gaston* Liquid metals as dynamic systems for atomically-precise control	*Daniel Escudero* Modelling intersystem crossing processes in thermally activated delayed fluorescence materials	*Daniel Crawford* Reduced-scaling coupled-cluster theory in the frequency and time domains	*Guido von Rudorff* Quantum alchemy: Treating chemical space with perturbations
15:00	*Oriol Vendrell* Vibrational, vibronic and electronic quantum dynamics with the MCTDH approach	*Yang Guo* Recent developments in multi-reference methods with large active space	*Natalie Gelfand* Integrative biochemical and simulation analysis of haloalkane dehalogenase mutants engineered by generative AI	*Aijun Du* Computational design of new materials for electronics, energy and environmental applications	*Michal Repisky* Relativistic real-time time-dependent density functional theory for valence and core attosecond pump-probe spectroscopic processes	*Miao Liu* Atomly.net: Paving a data-centric high-way for materials science
15:30-16:00	Coffee Break					

PROGRAM - TUESDAY, 15 October 2024

Time	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
16:00-18:00	ENDS Section 5 Chair: Tucker Carrington	DFT Section 3 Chair: Emmanuel Fromager	BIO Section 3 Chair: Steven Schwartz	MATER Section 3 Chair: Aijun Du	EMBED Section 2 Chair: Troy van Voorhis	SOFT Section 2 Chair: Edward Valeev
16:00	*Chun-Wei Pao* Multiscale molecular simulations of microstructure of ultraelastic chemically complex metals	*Andrew Teale* DFT reaction barriers: An adiabatic-connection perspective	*Jin Wang* Landscape and flux theory of biological systems	*Wenjie Dou* Floquet non-adiabatic dynamics for strong light-matter interactions near metal surfaces	*Tianyu Zhu* Towards systematic many-body treatment of excited-state phenomena in solids	*Hujun Qian* Success of treating topological dynamic propagation in polymer system with 1D Ising model: A novel full-scale dynamics-preserved coarse-grained polymer model
16:30	*Jianshu Cao* Transfer tensor method and applications to cavity polaritons	*Igor Ying Zhang* Toward efficient and unified treatment of static and dynamic correlations in generalized Kohn-Sham density functional theory	*Nadia Elghobashi-Meinhardt* Nature's strategy for small molecule capture and reduction: Investigating chemistry in iron-containing enzymes using quantum mechanics/molecular mechanics (QM/MM) and broken symmetry	*Linjun Wang* Mixed quantum-classical nonadiabatic dynamics methods and applications to large-scale semiconducting materials	*William Glover* Modelling photoinduced charge transfer with polarizable embedding	*Steven Kirk* The QuantVec software suite for next-generation QTAIM
17:00	*Seogjoo Jang* Fermi's Golden Rule rates for exciton transfer and nonradiative decay processes	*Neil Qiang Su* Hierarchically correlated orbital functional theory	*Wei Zhuang* Towards understanding the mechanism of the ultrafast dynamics of water hydrogen bonding network in bulk and interfaces	*Elena Besley* Crystal embedded multi-reference study of strongly correlated materials		*Zikuan Wang* New opportunities of photophysics and photochemistry studies using the BDF program
17:30	*Yi Zhao* Charge/energy transfer in organic aggregates simulated from stochastic Schrödinger equation	*James Patrick Lewis* FIREBALL2020: A revitalized paradigm for DFT molecular dynamics	*Yiqin Gao* Developing a molecular simulation package in connection with AI tools	*Xiaojun Wu* Visible-light-driven overall water splitting with covalent organic frameworks		*Jingxiang Zou* MOKIT: An open-source package that combines the strengths of existing quantum chemistry software
19:30-21:30	Hallway on the first floor (二楼会议中心走廊) Poster Session 2					

PROGRAM - WEDNESDAY, 16 October 2024

Time	Room 1 & 2, 1st floor (二楼会议中心)					
08:30-09:15	Plenary Lecture *Yundong Wu* Accurate and effective studies of peptide conformations and protein-peptide interactions				Chair: Yiqin Gao	
09:15-10:00	Plenary Lecture *Laura Gagliardi* Localized active spaces and quantum embedding for molecular and periodic systems				Chair: Trygve Helgaker	
10:00-10:30	Coffee Break					
	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
10:30-12:00	CAT Section 4 Chair: Anastassia Alexandrova	MLDD Section 4 Chair: Pavlo O. Dral	MATER Section 4 Chair: Weiqiao Deng	O(N) Section 2 Chair: Haibo Ma	EMBED Section 3 Chair: William Glover	QC4QC Section 2 Chair: Zhendong Li
10:30	*Jun Cheng* AI acceleration of AIMD simulation of dynamic catalysis	*Lipeng Chen* Efficient simulation of photo-induced dynamics processes and their spectroscopic characterization	*Momoji Kubo* Concerted phenomena on chemical reactions at nano-scale and mechanics at meso-scale in friction and wear processes revealed by large-scale molecular dynamics simulations	*Edward Valeev* Reduced-scaling coupled-cluster method using cluster-specific virtuals	*Christoph Jacob* Combining the many-body expansion and subsystem-DFT	*Rahul Maitra* Dynamic ansatz construction utilizing generative machine learning for molecular energetics in noisy quantum hardware
11:00	*Christopher Stein* Cluster embedding and a grand-canonical hybrid explicit/implicit solvation model for computational catalysis	*Jin Wen* Ultrafast dynamics simulations accelerated by machine learning models	*De-en Jiang* Understanding and predicting superionic Li-ion transport in amorphous halides	*John Herbert* Open-source framework for community validation of fragment-based quantum chemistry	*Michele Pavanello* Making and breaking electronic structures: lessons from embedding and machine learning	*Zhenyu Li* Quantum algorithms for electronic structure calculations
11:30	*Qian Peng* A theoretical perspective of spin control on iron-catalyzed reactions	*Arif Ullah* AI4Science: Quantum dissipative dynamics in the age of machine learning	*Karsten Reuter* Out of the crystalline comfort zone: Tackling working interfaces with machine learning		*Dingshun Lv* Towards realistic simulation of material with ab initio quantum embedding method	*Yuchen Wang* Simulating open quantum system dynamics on NISQ computers with generalized quantum master equations
12:00-13:30	Lunch Break					
13:00-18:30	Excursions					
18:30-21:00	Room 1 & 2, 1st floor (二楼会议中心) Conference Dinner					

PROGRAM- THURSDAY, 17 October 2024

Time	Room 1 & 2, 1st floor (二楼会议中心)					
08:30-09:15	Plenary Lecture *Eberhard K.U. Gross* Non-adiabaticity from first principles: The exact factorization				Chair: Edward Valeev	
09:15-10:00	Plenary Lecture *Jiali Gao* Multistate density functional theory and applications				Chair: Shuhua Li	
10:00-10:30	Coffee Break					
	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
10:30-12:00	ENDS Section 6 Chair: Mark Tuckerman	CAT Section 5 Chair: Sergey Kozlov	DFT Section 4 Chair: Ilaria Ciofini	O(N) Section 3 Chair: Shuhua Li	SPECT Section 5 Chair: Trygve Helgaker	SOFT Section 3 Chair: Wei Hu
10:30	*Zlatko Bačić* Water trimer: Intermolecular vibration-tunneling states and low-frequency spectrum from high-dimensional quantum calculations	*Luigi Cavallo* NHC-cracker: A platform for the engineering of N-heterocyclic carbenes for diverse chemical applications	*Wei Wu* Multireference density functional theory with valence bond methods	*Michael Dolg* From crystalline solids to molecules: The incremental scheme for ab initio electron correlation energy estimates	*Robert Berger* Computational spectroscopy for precision experiments: From electroweak to quantum electrodynamical effects	*Qiming Sun* GPU acceleration in PySCF
11:00	*Yijing Yan* Dissipatons as generalized Brownian particles in open quantum systems	*Ming Lei* Mechanism-based organometallic catalyst design: A hole in the ice	*Chen Li* Improving density functional approximations through exact constraints and exact wave function	*Yuriko Aoki* Recent development of elongation method and its applications toward functional designs	*Christoph van Wüllen* Quantum Chemical Calculation of ^{193}Ir Mössbauer Spectra	*Jun Zhang* Target state optimization density functional theory
11:30	*Jiří Vaníček* Vibronic spectra at nonzero temperatures from coherence thermofield dynamics	*Andrew Rappe* Stretching the limits of surface reactivity: Mechanochemistry and topological catalysis	*Timothy Gould* Accurate ΔSCF from ensemble density functional theory	*Ganglong Cui* Efficient fragment-based electronic structure methods for excited states		*Youliang Zhu* A molecular dynamics simulation software for polymers
12:00-13:30	Lunch Break					
12:50-13:20	Sponsor Lecture: Room 4, *Jun Jiang (AI-chem),* 理实交融的机器化学家平台					

PROGRAM - THURSDAY, 17 October 2024

Time	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
13:30-15:30	ENDS Section 7 Chair: Zhonghan Hu	WFT Section 4 Chair: Pierre-François Loos	CAT Section 6 Chair: Jun Cheng	BIO Section 4 Chair:Yaoqi Zhou	MATER Section 5 Chair: Yuchen Ma	MLDD Section 5 Chair: Jacqueline Cole
13:30	*Mark Tuckerman* Synthesizing first-principles simulation, machine learning, and experimental strategies for the design and analysis of a new class of high-performance battery electrolytes exploiting the Grotthuss structural diffusion mechanism	*Piotr Piecuch* Converging high-level coupled-cluster energetics with semi-stochastic, CIPSI-driven, and adaptive CC(P; Q) methods	*Zhipan Liu* Machine-learning atomic simulation resolves active site for selective ethene epoxidation on silver	*Steven Schwartz* Transition Path Sampling studies of the evolution of reactions in enzymes	*Weiqiao Deng* Digital-intellectual materials design	*Guanhua Chen* Improving the accuracy of density functional theory via Δ-learning and machine-learning exact exchange-correlation functional
14:00	*Maxim Gelin* Ab initio doorway-window methods for the simulation of nonlinear s pectroscopic signals	*Feiwu Chen* Recent progress on the multireference electronic structure theory	*Mikhail V. Polynski* Advancing realism in catalytic models: Modeling active sites on nanoparticles	*Barak Hirshberg* Combining resetting with metadynamics for improved sampling and kinetics inference	*Krzysztof Szalewicz* Reliable predictions of crystal structures entirely from first principles	*Jun Jiang* A data driven robotic AI-chemist
14:30	*Samantha Jenkins* Ultrafast processes: A next generation QTAIM interpretation	*Katharina Boguslawski* Alternative coupled cluster methods based on electron-pair theories	*Jilai Li* Electronic effects on gas-phase C-H bond activations by cluster oxides and metal carbides: The methane challenge	*Jing Huang* Identifying most probable transition path with constant advance replicas	*Dongwook Kim* Chemical stabilities of OLED materials in the excited states: A DFT study	*Milica Todorović* Active learning for surface adsorption chemistry
15:00	*Michał Tomza* Quantum control of ultracold atom-ion and atom-molecule collisions	*Jiří Pittner* DMRG-tailored coupled cluster method in the 4c-relativistic domain	*Xiaojing Liu* Theoretical design of energy catalysis	*Wenning Wang* Molecular mechanism of channel transport: From synthetic channels to protein		
15:30-16:00	Coffee Break					

PROGRAM - THURSDAY, 17 October 2024

Time	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
16:00-18:00	DFT Section 5 Chair: Igor Ying Zhang	WFT Section 5 Chair: Katarzyna Pernal	Relativity Section 2 Chair: Eugene DePrince	BIO Section 5 Chair: Wei Zhuang	QC4QC Section 3 Chair: Junxu Li	
16:00	*Ilaria Ciofini* Tuning Range Separated Hybrids for the description of excited states	*Mark R. Hoffmann* Downfolding in atomic and molecular electronic structure	*André Severo Pereira Gomes* Core and valence properties of heavy element species from relativistic (embedded) coupled cluster calculations	*Yaoqi Zhou* RNA-MobiSeq: Deep mutational scanning and mobility-based selection for RNA 2D & 3D structure inference	*Kosuke Mitarai* Beyond VQE methods for quantum chemistry on quantum computers	
16:30	*Cheol Ho Choi* Advancements in MRSF-TDDFT: Addressing the limitations of DFT/TDDFT	*Mihály Kállay* Basis-set limit correlation energies for large molecules with density-based basis-set corrections	*Jing Su* Theoretical studies of coordination structures and electronic spectra of Cm3+ species at the mineral-water interface	*Pietro Faccioli* Physiological and pharmacological role of protein folding pathways	*Xiao Yuan* Quantum computational chemistry	
17:00	*Eduard Matito* Modern density functional approximations are ill-designed to compute molecular properties	*Thomas Jagau* Complex-scaled electronic-structure methods for nonradiative decay processes	*Minori Abe* Development and application of a relativistic CASPT2/RASPT2 program based on the DIRAC software	*Hao Wang* Modeling and analyzing long-time dynamics in complex systems	*Zixuan Hu* A general quantum algorithm for simulating open quantum dynamics	
17:30	*Bruno Senjean* Density functional theory on quantum computers	*Ke Liao* Quantum-information-based orbital optimization, energy-filtered excited states and electron dynamics within the coupled cluster framework		*Jun Gao* Multi-scale simulation of photosynthesis system		
19:30-21:30	Hallway on the first floor (二楼会议中心走廊)					
	Poster Session 3					

PROGRAM- FRIDAY, 18 October 2024

Time	Room 1, 1st floor (会议中心前区)	Room 2, 1st floor (会议中心后区)	Room 3, 1st floor (二楼会议厅)	Room 4, 2nd floor (3 楼第二会议室)	Room 5, 3rd floor (4 楼锦绣厅)	Room 6, 20th floor (21 楼云帆阁)
08:30-10:00	WFT Section 6 Chair: Yang Guo	DFT Section 6 Chair: Xin Xu	MLDD Section 6 Chair: Jin Wen	EMBED Section 4 Chair: Hong Jiang	Relativity Section 3 Chair: André Severo Pereira Gomes	MEM Section 3 Chair: Odile Eisenstein
08:30	*Pierre-François Loos* Green's function methods for quantum chemistry	*Juan Felipe Huan Lew-Yee* Towards efficient calculations of strongly correlated systems with natural orbital functional theory	*Dongqing Wei* AIDD and drug candidates by super-computing: Anti-Aging, Cancer and Covid-19	*Matthew Hermes* LASSIS: a general model space recipe for two-step diagonalization of multimetallic molecular wave functions	*Eugene DePrince* Relativistic equation-of-motion coupled-cluster for single and double ionization	*Krzysztof Szalewicz* Remembering Bogumil Jeziorski and his breakthrough insights in theory of intermolecular forces
09:00	*Andreas Grüneis* Resolving shortcomings of CCSD(T) theory for metals and large molecules	*Fenglong Gu* TDDFT/TDHF Methods Based on Non-Orthogonal Localized Molecular Orbitals and Its Applications	*Hanshi Hu* Ab initio molecular dynamics simulation of fullerene-like and graphene-like uranyl materials	*Tomasz A. Wesolowski* Approximating the bi-functional of the nonadditive kinetic potential for frozen-density embedding theory based multi-level simulations	*Xiaoyan Cao* Pseudopotential studies on the complexation of Uranyl with Fluoride	*Piotr Piecuch* Remembering Professor Josef Paldus: Pioneer of modern electronic structure theory and caring mentor, educator, and friend
09:30	*Zhenhua Chen* Diabatic electronic-structure theory: Method development and its applications in analyzing chemical reactivity	*Jan M. L. Martin* Minimally empirical double hybrids: A status update	*Lin Shen* Long short-term memory networks for surface hopping dynamics simulations of photochemical reactions	*Lyudmila Slipchenko* TBA	*Xiaosong Li* Over-destabilization vs. over-stabilization in theoretical analysis of f-orbital covalency	*Hui Li* Remembering Professor Auchin Tang: Pioneer and founder of modern theoretical chemistry in China and outstanding educator
10:00-10:30	Coffee Break					
Time	Room 1 & 2, 1st floor (二楼会议中心)					
10:30-11:15	Plenary Lecture *Debashis Mukherjee* Spin adapted multireference correlation methods for construction of potential energy curves (PECs)				Chair: Mark R. Hoffmann	
11:15-12:00	Closing Ceremony				Chair: Wenjian Liu	

POSTER SESSIONS

Poster Session 1 – 19:30-21:30, Monday, 14 October 2024

PO1-1	Highly coarse-grained patchy ellipsoid particle model of glucose	Bin Li
PO1-3	Atomistic insights on recognition of transcription factor binding motif in DNA through bZIP domain	Piya Patra
PO1-4	Structure and catalytic properties of Cu-Au nanoparticles under high CO and O coverage	Anastasiia Mikhailova
PO1-5	Computational screening of doped-$V_3C_2O_2$ for propane dehydrogenation using DFT-based microkinetic simulations	Aqsa Abid
PO1-6	Modeling realistic structures of trimetallic nanoalloy catalysts using chemically meaningful descriptors	Arravind Subramanian
PO1-7	Accurate adsorption energy predictions using many-body methods with quantum embedding	Changsu Cao
PO1-8	TBA	Congqiao Xu
PO1-9	Illuminating tandem reactions characterized by temporal separation of catalytic activities via DFT calculations: A case study of Ni-catalyzed alkyne semihydrogenation	Dongju Zhang
PO1-10	Effect of ZnO support and nanostructuring on catalytic activity of noble metals: Insights from Sabatier principle	Fernando Buendia Zamudio
PO1-11	Theoretical insights into the ammonia and hydrogen-induced structural evolution of Pt clusters in mordenite	Gang Feng
PO1-12	Mean-field QM/MM simulations for electrochemical interfaces	Hyungjun Kim
PO1-13	Structure-driven tuning of adsorption properties of core-shell nanoparticles: a density functional theory study	Ilia Chepkasov
PO1-14	Controlling active phase and interface interactions in bimetallic Ru-Pd catalyst via CO oxidation	Janobiddinkhuja Bahodurov
PO1-15	Delayed fluorescence from inverted singlet and triplet excited states in heptazine analogues HzT-FEX2 studied by mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT)	Alireza Lashkaripour
PO1-16	Advances in Q-Chem 6.2	Andrew Gilbert
PO1-17	Extension of the charge stabilization method beyond energies	Charlotte Titeca
PO1-18	Noncollinear functionals for real-time TDDFT and gradients of spin-flip TDDFT	Hao Li
PO1-20	Unraveling the mechanism of a switchable acid catalyzed COT oxide contraction towards homoallylic alcohols	Manuel Pedrón

PO1-21	Some restrictive open-shell excited-state ΔSCF methods	Peng Bao
PO1-22	Electronic structure of periodic systems containing strongly correlated transition metals	Ilya Popov
PO1-23	Density-based many-body expansion as a case study on interoperability	Kevin Focke
PO1-24	Developments of approaches for structural relaxation of excited states of materials based on embedded cluster model	Teng Zhang
PO1-25	Nonadiabatic field on quantum phase space	Baihua Wu
PO1-26	Mechanistic insights into twisted intramolecular charge transfer in CBP and its derivatives	Donghwan Im
PO1-27	Building accurate molecular simulation models for studying warm cloud seeding	Guangzhi He
PO1-28	Correlation functions from tensor network influence functionals: The case of the spin-boson model	Haimi Nguyen
PO1-29	Time-dependent density matrix renormalization group method for quantum transport with phonon coupling in molecular junction	Hengrui Yang
PO1-30	Solvated electron from first principles and machine learning	Jinggang Lan
PO1-31	Real-time time-dependent density functional theory for X-ray absorptions	Linfeng Ye
PO1-32	A stochastic Schrödinger equation and matrix product state approach to carrier transport in organic semiconductors with nonlocal electron-phonon interaction	Liqi Zhou
PO1-33	Non-unique Hamiltonians for discrete symplectic dynamics	Liyan Ni
PO1-34	An electronic spin on geometric phase effects in molecular systems	Martin van Horn
PO1-35	Excursions in polaritonic chemistry: From relaxation in liquids to chemical kinetics	Muhammad Risyad Hasyim
PO1-36	Early stages of battery electrolytes degradation: Theory and experiment	Alia Tadjer
PO1-37	Stability and ion conductivity of novel Li_6PIO_5 : A DFT study	Areg Hunanyan
PO1-38	Disordered structure reduces the bandgap of double perovskite Cs_2 AgBiBr$_6$ t hrough wavefunction localization	Bayan Amer Abzakh
PO1-39	A theoretical study on proton transfer reactions in anthracene-urea derivatives	Changbang Long
PO1-40	Theoretical study on the effect of ring modification in cuprous halide complexes on the TADF mechanism	Guangyu Wang
PO1-41	Review on improving the performance of SiOx anodes for a lithium-ion battery through insertion of heteroatoms: State of the art and outlook	Hai Li
PO1-42	Theoretical study on singlet fission dynamics in finite-size molecular aggregates with various intermolecular interaction strengths and structures	Hajime Miyamoto
PO1-43	A molecular dynamics simulation on the stress corrosion cracking mechanism of BCC-FCC type dual-phase high-entropy alloys	Haoyu Zhao

PO1-44	Modelling of sodium clusters in various conjugated carbonaceous structures	Hristo Rasheev
PO1-45	Assessing short-range charge transfer character of potential MR-TADF emitters with wavefunction descriptors	Mariana Telles do Casal
PO1-46	XEDA: An efficient and flexible energy decomposition analysis (EDA) toolkit	Yueyang Zhang
PO1-47	Sub- and supercritical water structure calculated using the self-learning path integral hybrid Monte Carlo method	Bo Thomsen
PO1-48	Towards ML- and QML-accelerated discovery of catalytic materials and mechanisms	Dennis Salahub
PO1-49	Breaking the size limitation of non-adiabatic molecular dynamics in condensed matter systems with local descriptor machine learning	Dongyu Liu
PO1-50	Reciprocal prediction of multimodal spectral and structural descriptors for incomplete data	Guokun Yang
PO1-51	Spectra-based clustering of high-entropy alloy catalysts: Improved insight over use of atomic structure	Huirong Li
PO1-52	A simple approach to rotationally invariant machine learning of a vector quantity	Jakub Martinka
PO1-53	Machine learning photodynamics uncover blocked non-radiative mechanisms in aggregation-induced emission	Jingbai Li
PO1-54	Density functional theory and machine learning exploration of disorder in materials	Jingrui Li
PO1-55	Stochastic resolution of identity to CC2 for large systems	Chongxiao Zhao
PO1-57	Quantum simulation with cluster embedding strategy for surface chemisty	Dedong Wan
PO1-59	Development of a compact and dynamic ansatz for enhanced quantum efficiency	Dipanjali Halder
PO1-60	Nuclear quantum effects enhance hydrogen evolution reaction on graphene-embedded transition metal atoms	Erxun Han
PO1-61	Development of quantum embedding computing for Quantum Chemistry	Wafa Makhlouf
PO1-62	Chemoexcited formation and radiationless decay dynamics of firefly chromophore	Maryam Farmani
PO1-63	Theoretical study of lanthanide single-ion magnet: Electronic structure, magnetic anisotropy and relaxation	Bing Yin
PO1-64	The automated design of chemical reactions program	Guoao Li
PO1-65	A workflow for reaction datasets construction by layer-based modification modeling process.	Hexiang Qi
PO1-66	Mapping hydrogen positions along proton transfer pathway in organic crystals by computational X-ray spectra	Guoyan Ge

PO1-67	A Green's-function-based many-body perturbation theory approach to electron-vibration coupling in molecular systems	Haoyu Qi
PO1-68	Reveling the ultrafast energy transfer pathways in energetic materials: Time-dependent and quantum state-resolved	Jia Liu
PO1-69	Second-order Møller–Plesset perturbation theory with pair natural orbitals for periodic systems	Andrew Zhu
PO1-71	Equation-of-motion block-correlated coupled cluster method for excited electronic states of strongly correlated systems	Haodong Zhang
PO1-72	Toward a systematic and high-precision ab initio framework for metallic solids	Hung Pham
PO1-73	The truncation schemes for unitary coupled-cluster based polarization propagator theory	Junzi Liu
PO1-74	A moiety-based charge-transfer decomposition for exploring the charge-transfer character and exciton binding energies in dye-sensitized solar cells	Lena Szczuczko
PO1-75	DC-MP2-PBC: Fast and accurate quantum chemical calculation for large-scall periodic systems	Ogawa Gen
PO1-76	Unveiling the local structure of liquid water via X-ray spectroscopy simulations employing multiconfigurational wave function theory	Alekos Segalina
PO1-77	U≡C triple bonds in fullerene compounds	Jing Zhao
PO1-78	Design strategy of MR-TADF materials with tunable Stokes shift and narrow spectra band through-space conjugation	Meihui Liu
PO1-79	Million-atom molecular dynamics simulations on the splitting mechanism of Ni particles within the anode of solid oxide fuel cells	Yixin Su
PO1-80	Relativistic effects in ultrafast light induced spectroscopy	Torsha Moitra
PO1-81	Time evolving matrix product operator (TEMPO) method in a non-diagonal basis set based on derivative of the path integral expression	Shuocang Zhang
PO1-82	MC23: A New Meta-GGA On-Top Functional for Hybrid Multiconfiguration Pair-Density Functional Theory with Improved Accuracy	Jie Bao

Poster Session 2 – 19:30-21:30, Tuesday, 15 October 2024

PO2-1	Rare event kinetics in complex systems with Milestoning	Ru Wang
PO2-2	How transcription factor NF-κB RelA recognize a central base pair: Computational insights into transient interactions	Tianjie Li
PO2-3	Accurate carbohydrate-binding site prediction	Xi Cheng
PO2-4	Probing the orientation and membrane permeation of Rhodamine Voltage Reporters through molecular dynamics and free energy calculations	Yajing Qi
PO2-5	CO_2 t o methanol conversion on Cu/ZnO catalyst: Unveiling the role of catalyst architecture and binding affinity	Jie Zhao
PO2-6	Tailoring active-site spacing of single-atom catalyst for CH_4-to-CH_3O H conversion: Co_1/UiO-66 MOF as an exemplary model	Karim Harrath
PO2-7	Inverted region in electrochemical reduction of CO_2 i nduced by potential-dependent Pauli repulsion	Leyu Liu
PO2-8	Effective screening descriptors of metal−organic framework supported single-atom catalysts for electrochemical CO_2 reduction reactions	Lihui Mou
PO2-9	Towards systematic initiations of minimum energy path calculations	Maike Muecke
PO2-10	A theoretical study on the asymmetric site of CO_2 h ydrogenation to methanol on Cu-based catalysts	Mingcan Chen
PO2-11	CO_2 e lectroreduction to CO on ultrasmall Ag nanoparticles supported on polymeric carbon nitride (PCN)	Mohammed Aliasgar
PO2-13	The oxidation of CO on step interfaces between ZnO deposits and metal supports	Paulo de Carvalho Dias Mendes
PO2-14	Small molecule activation by uranium and group 6 metal complexes, a theoretical study	Qingjiang Pan
PO2-16	Explicitly density-dependent noncollinear and nonlocal exchange-correlation functional	Tai Wang
PO2-17	A tuning method for range-separated hybrid functionals based on charge transfer density-based indexes	Tianhong Yan
PO2-18	Energetic information from information-theoretic approach in density functional theory as quantitative measures of physicochemical properties	Xin He
PO2-19	Exact properties of multi-state density functional theory	Yangyi Lu
PO2-20	Exploring the range-separation schemes in the range-separated hybrid functionals	Ye Li

PO2-21	Towards consistent projection-based wavefunction in density functional theory embedding	Yitian Zhu
PO2-22	Comparison of solvent electrostatic potential and improvement proposal for polarizable continuum model	Yuki Kanamaru
PO2-23	Role of electronic polarization in the primary charge-transfer states of the purple bacteria reaction center: A polarizable QM/MM study with the integral-exact direct reaction field method	Yuquan Cao
PO2-24	Application of quantum embedding theory on lanthanide-based materials	Zewei Li
PO2-25	Excitonic energy transfer under strong coupling from a semi-classical surface hopping perspective	Priyam Kumar De
PO2-26	Ab-initio study on the effect of dipolar spin-spin interactions in singlet fission	R. K. Kathir
PO2-27	Radiosensitizing potential of halo-uracils via low-energy electrons: A simulation study	Raj Roy
PO2-28	Describing nuclear quantum effects in coupled nuclear-electron dynamics at gas-metal surface: A ring polymer molecular dynamics extension to electronic friction	Ruihao Bi
PO2-29	First-principles demonstration of nonadiabatic Thouless pumping of electrons in a molecular system	Ruiyi Zhou
PO2-30	A grid-based gauge-invariant non-perturbative solution of the Schrodinger equation for electrons and nuclei in strong magnetic fields	Sangita Sen
PO2-31	Non-adiabatic molecular dynamics on ultrafast relaxation of ortho-nitrophenol upon photoexcitation	Satoi Wada
PO2-32	Theoretical study of the spin transition processes of molecular systems	Shuming Bai
PO2-33	Phonon-mediated ultrafast energy- and momentum-resolved hole dynamics in monolayer black phosphorus	Siyuan Gao
PO2-34	Large-scale nonadiabatic dynamics study of doping process within PbSe quantum dots	Tenghui Li
PO2-35	Multi-scale modeling of hydroxyl radical reactions with isoprene in the gas phase and at the air-water interface	Tianren Zhu
PO2-36	Ab initio investigation of the features of $Sr_3Ti_3(BO_6)_2$	Mikayel Sahakyan
PO2-37	Study of the influence of the grain boundary structure on the properties of $CsPbBr_3$ perovskite	Mikhail Samatov
PO2-38	Time-domain ab initio analysis of facet-dependent carrier dynamics in Cuprous oxide	Minjae Kwen
PO2-39	Mechanism of lithium dendrite growth on iron surfaces toward high-performance and safe anode-free lithium metal batteries	Nannan Li
PO2-40	Computational screening of multi-resonance thermally activated delayed fluorescence (MR-TADF) molecules for lasing application	Rongrong Li
PO2-41	Theoretical study on open-shell electronic structures of through-bond through-space hybrid conjugated systems	Ryohei Kishi

PO2-42	Computational study on high-performance memristors utilizing nanomanipulation and device architecture design	Shuang Chen
PO2-43	Theoretical studies of 0D-perovskite based luminescent materials	Songqi Cao
PO2-44	Intrinsic defects in B- site columnar-ordered halide double perovskites Cs_2 AgPdBr_5	Wenjun Chu
PO2-45	Growth kinetics of single-crystal covalent organic frameworks	Xiangkun Yu
PO2-46	Do Zimmermann-Traxler transition states always have strong explanatory power? --A combined experimental and computational 'archaeology of chemistry' study.	Zongchang Han
PO2-47	Analysis of organic reactions by combinatorial optimization and dimension reduction method	Lihao Qu
PO2-48	Mechanistic insights into water autoionization through metadynamics simulation enhanced by machine learning	Ling Liu
PO2-49	Enhancing molecular data through quantum chemical calculations: An overview of the PubChemQC project	Maho Nakata
PO2-50	Predicting heat capacity of molecular fluids using interpretable machine learning models: Application of the Fluid_Thermo database	Simin Li
PO2-51	Scalable and accurate chemical property predictions using universal neural network potentials as atomic descriptors	Tomoya Shiota
PO2-52	Machine learning force field construction of organmetallic complex materials: An equilibrium molecular dynamics study on thermal conductivity calculation of copper phthalocyanine	Wenjie Zhang
PO2-53	Development of programs for identifying active sites on catalyst surfaces and constructing databases for transition states	Xiao Ma
PO2-54	An AI-assisted pure density-based nonlocal functional	Xiaoyu Zhang
PO2-55	Fragment-based deep learning for simultaneous prediction of polarizabilities and NMR shieldings of macromolecules and their aggregates	Dongbo Zhao
PO2-56	Unveiling the impact of the air-water interface on altering reaction mechanisms: Incorporating DFT, AIMD, and CMD	Mohammad Hassan Hadizadeh
PO2-58	Calculating potential energy surfaces with the variational quantum eigensolver	Shizheng Zhang
PO2-59	Enhancing variational quantum eigensolver with clifford transformation and robust parameter optimization	Weitang Li
PO2-60	Grid-based quantum simulation of photoexcited pyrazine	Xiaoning Feng
PO2-61	The application of Hardware heuristic ansatz in periodic system	Xiaopeng Li
PO2-62	How to experimentally detect planar tetracoordinate hydrogen within the indium framework? An answer from quantum dynamics theory	Xingyu Zhang

PO2-63	Uranium dioxide-mediated carbon dioxide photoreduction	Xuelian Jiang
PO2-64	Automated review generation method based on large language models	Shican Wu
PO2-65	Coupling simulations of spatiotemporal electromagnetic fields with simulations of ultrafast photoinduced dynamics	Lorenz Grünewald
PO2-66	Femtosecond pump-probe-spectra in the heptazine-H_2O complex: A computational study	Sebastian Viktor Pios
PO2-67	Simulating transient X-ray spectra of molecules and crystals from snapshots along the potential energy surfaces	Weijie Hua
PO2-68	Accurate and efficient NMR shielding calculation with parallel, fully RI-boosted finite 1st derivative framework	Xiao Liu
PO2-69	Linear response pCCD-based methods	Paweł Tecmer
PO2-70	Individual and cooperative superexchange enhancement in cuprates	Tonghuan Jiang
PO2-71	Block-correlated coupled cluster theory for accurate static correlation of strongly correlated systems	Xiaochuan Ren
PO2-72	Excitonic model for excited state processes in molecular aggregate	Xiaoyu Xie
PO2-73	When do tripdoublet states fluoresce? A theoretical study of copper(II) porphyrin	Xingwen Wang
PO2-74	QUEST#4X: an extension of QUEST#4 for benchmarking multireference wavefunction methods	Yangyang Song
PO2-75	Triple electron attachments with a new Intermediate-Hamiltonian Fock-space coupled-cluster method	Yanmei Hu
PO2-76	Exhaustive screening of topological high-fold degenerate semimetal with chiral structure	Yan Wang
PO2-77	Magnetic topological Weyl fermions in half-metallic In_2CoSe_4	Qiunan Xu
PO2-78	The description of atom and bond reactivity in the language of conceptual density (matrix) functional theory	Bing Wang
PO2-79	Structure and dynamics at Pt/water interfaces revealed by machine learning molecular dynamics	Feiteng Wang
PO2-80	Dimensionality reduction in electronic structure theory via nonlinear dynamics and machine learning: Classical and quantum computing aspects	Chayan Patra
PO2-81	Multivalent interactions in sequence mediated spontaneous association of short RNA chains	Manas Mondal
PO2-82	Quantitative Studies of the Key Aspects in Selective Acetylene Hydrogenation on Pd(111)	Wenbo Xie

Poster Session 3 – 19:30-21:30, Thursday, 17 October 2024

PO3-1	Multiscale regulation of light-harvesting and quenching in LHCII protein	Yingjie Wang
PO3-2	Long-range electron tunneling through protein junctions	Zdenek Futera
PO3-3	Accelerating reliable multiscale quantum refinement of protein–drug systems enabled by machine learning	Zeyin Yan
PO3-4	ReaxFF force field parameter optimization based on enhanced sampling algorithm	Shuang Li
PO3-5	Stability of Ru@Sn_9 Z intl cluster on a CeO_2 (111) surface and its catalytic activity in Water-Gas-Shift (WGS) reaction.	Sourav Mondal
PO3-6	Theoretical investigation of Fe-based perovskite for chemical looping partial oxidation of methane	Tingting Yang
PO3-7	Importance of material surface structure for photocatalytic reactions in water	Wenhui Ding
PO3-8	Computational insights into how Co/Mn dopants stabilize RuO_2 catalyst under OER conditions	Wenrui Ma
PO3-9	Theory-driven catalyst design for propane dehydrogenation	Xin Chang
PO3-10	Properties of metal-supported ZnO films and their application in water splitting	Yizhen Song
PO3-11	Kinetic simulations of methanol steam reforming and CO_2 h ydrogenation	Yongjie Jiang
PO3-12	How to achieve both stability and activity in Fe-N-C electrocatalysts for ORR: Unifying roles of O and S doping	Yuan Yuan
PO3-13	Efficient and flexible approach for local distortion: Distortion distribution analysis enabled by fragmentation	Yunteng Liao
PO3-14	The role of bases and silver(I) additives in the ligand-promoted β-C(sp^3)-H heteroarylation of free carboxylic acids	Zhewei Li
PO3-15	Noncollinear functional construction schemes in different dimensions	Yu Jing
PO3-16	From collinear functionals to noncollinear functionals	Yunlong Xiao
PO3-17	Exact constraint of density functional approximations at the semiclassical limit	Yunzhi Li
PO3-18	A pointwise machine learning correction to eliminate error cancellation in density functional approximation	Zipeng An
PO3-19	Snap-shots of cluster growth: Electronic structures of a Zintl ion with a linear Fe_3 core, $[Fe_3Sn_{18}]^{4-}$	Zisheng Li
PO3-20	Exact factorization-based density functional theory beyond the Born-Oppenheimer approximation: Case study of a model system	Zixuan Wang
PO3-21	Dynamic correlation in single-ion magnets using density matrix embedding theory	Zhebin Guan

PO3-22	Dynamical mean-field theory of the Holstein polaron: Solving the impurity Green's function by discretizing the hybridization function	Zhecun Shi
PO3-23	Towards realistic simulation of material with ab-initio correlated method	Zigeng Huang
PO3-25	Dual-mode floquet quantum master equation for electronic transport in a bichromatic-driven quantum dot	Vahid Mosallanejad
PO3-26	Machine learning assisted first-principles simulation of tunneling phenomena in spectroscopy	Wei Fang
PO3-27	Memory kernel coupling theory: Obtain time correlation function from higher-order moments	Wei Liu
PO3-28	New insights into phase space representations for finite-state quantum systems and applications in nonadiabatic transition dynamics	Xiangsong Cheng
PO3-29	The exact solution to the finite size one dimension model	Yang He
PO3-30	Theoretical analysis of X-ray spectra of water	Yihao Zhao
PO3-31	Stability of quantum systems beyond canonical typicality	Yu Su
PO3-32	Mechanisms of the interlayer charge transfer in two-dimensional heterostructures: nonadiabatic molecular dynamics investigations	Yuli Lei
PO3-33	The electronic friction effects of strongly correlated systems	Yunhao Liu
PO3-34	Photo-induced dynamics with continuous and discrete quantum baths	Zhaoxuan Xie
PO3-35	TD-DMRG study of exciton dynamics with both thermal and static disorders for Fenna-Matthews-Olson complex	Zirui Sheng
PO3-36	Theoretical calculation of organic host-guest doped materials with room temperature phosphorescence	Xiaoli Wang
PO3-37	Hierarchical approximation and question-driven strategy for efficient computation of charge transport in molecular devices	Xuan Ji
PO3-39	Design of bipolar organic matrices for rechargeable redox reactions in non-aqueous electrolytes	Yanislav Danchovski
PO3-40	Device engineering optimization of organic photovoltaic assisted by machine learning	Yaping Wen
PO3-41	Theory of electron spin resonance spectroscopy in scanning tunneling microscopy	Lyuzhou Ye
PO3-42	Modelling the emissive properties of NIR-emitters	Yixuan Li
PO3-43	Simultaneous intra- and intermolecular singlet fission through macrocyclic structures	Zhangxia Wang
PO3-44	PM6/L8-BO thin films through layer-by-layer engineering: Formation mechanism, energetic disorder, and carrier mobility	Zihao Wen
PO3-45	Machine learning-assisted dual-atom sites design with interpretable descriptors unifying	Xiaoyun Lin

PO3-46	DPA-Semi:Machine-learning-based interatomic potentials for group IIB to VIA semiconductors: Towards a universal model	Xingchen Zhang
PO3-47	Machine learning-aided in-situ structure identification of low-dimensional carbon nanomaterials from STM images	Yanbo Li
PO3-48	Predicting regioselectivity in functionalized fullerenes and carboncones using deep learning	Yang Wang
PO3-49	Active learning for fast and robust dynamics simulations	Yifan Hou
PO3-50	Stability prediction of gold nanoclusters with different ligands and doped metals by deep learning	Yuming Gu
PO3-51	UAIQM – the new generation of universal AI models	Yuxinxin Chen
PO3-52	Performance prediction for all small-molecule-based organic solar cells	Zhiwen Zhao
PO3-53	DC-PUHF: Toward large-scale quantum chemical calculation including static correlation	Masatsugu Nishida
PO3-54	Accurate and efficient CCSD(T)/CBS: Development and application for complicated molecules up to 1000 atoms	Peter Nagy
PO3-55	Accurate chemical reaction modeling on noisy intermediate-scale quantum computers using a noise-resilient wavefunction ansatz	Xiongzhi Zeng
PO3-56	Variational quantum computation for large molecules using matrix product state inspired ansatz	Yi Fan
PO3-57	Quantum equation-of-motion method with triple excitations reduced by perturbation and symmetry	Yuhan Zheng
PO3-58	Quantum structure search for molecular ground-state energy computation	Yunong Li
PO3-59	A hybrid framework for simulating molecular systems on quantum computers	Zhanou Liu
PO3-60	Integrating self-initialized local thermalizing lindblad operators for variational quantum algorithm with quantum jump: Implementation and performance	Zhihao Lan
PO3-61	Circuit-efficient Qubit-excitation-based variational quantum eigensolver	Zhijie Sun
PO3-62	Kylin-V: An open-source package calculating the dynamic and spectroscopic properties of large systems	Yihe Xu
PO3-63	Metal-centered boron-wheel cluster of $Y©B_{11}^{2-}$ with rare D_{11h} Symmetry	Xinran Dong
PO3-64	Theoretical studies on strong coupling mechanism between surface plasmon and molecules	Xueyang Zhen
PO3-65	Analytical derivative approaches for vibro-polaritionic structures and properties	Xunkun Huang
PO3-66	Electronic absorption and circular dichroism spectra of one-dimensional bay-substituted chiral PDIs: Effects of intermolecular interactions, vibronic coupling and aggregate size	Yuchuan Xu
PO3-67	Quantum chemical approaches based on renormalized states for strongly correlated systems	Yifan Cheng
PO3-68	Towards an exact description of Compound I in P450	Yifei Huang

PO3-69	Parallel and GPU-accelerated implementation of density matrix renormalization group	Yingqi Tian
PO3-70	Kylin 1.2: An advanced ab-initio density matrix renormalization group program	Yinxuan Song
PO3-71	A multi-reference random phase approximation theory	Yuqi Wang
PO3-72	Diffusion quantum Monte Carlo studies multi-reference systems	Zhiru Huang
PO3-73	Exact analytic solutions of Schrödinger equations with non-separable variables: A case study of 1D quartic potential	Zhiyuan Yin
PO3-74	Formally exact and practically useful analytic solution of harmonium	Wenqing Yao
PO3-75	Distinct single-electron actinide−actinide bonding and fullerene-enhanced magnetism in two-dimensional diactinide endohedral metallofullerene monolayers	Xiaokun Zhao
PO3-76	Molecular descriptors for high-throughput screening of inverted singlet−triplet gap materials	Yu Pang
PO3-77	Employing uncertainty-driven active learning strategies to construct full-dimensional intermolecular potential energy surfaces within spectroscopic accuracy	You Li
PO3-78	Learning molecular conformational energies using semi-local density fingerprints	Zhuofan Shen
PO3-79	Development of a compact Ansatz via operator commutativity screening to avoid local traps and barren plateaus	Dibyendu Mondal
PO3-80	Tools for Overcoming Reliance on Energy-Based Measures in Chemistry: a Tutorial Review	Tianlv Xu
PO3-81	Response of the Mechanical and Chiral Character of Ethane to Ultra-Fast Laser Pulses	Tianlv Xu
PO3-82	Ultra-fast laser pulses as a probe of electron dynamics:A next generation QTAlM perspective	Huan He
PO3-83	Chirality reversal with the carrier-envelope phase: A next generation QTAlM interpretation	Xinjie Zhou

USEFUL INFORMATION

ISTCP

The International Society of Theoretical Chemical Physics (ISTCP) was founded by Janos Ladik in 1990 and is currently coordinated by President Erkki Brändas and Vice Presidents Leticia Ganzález, Peter Gill, Anna Krylov, and Mark R. Hoffman. The major activity of ISTCP is to organize a triennial congress to showcase the achievement and advances in theoretical chemical physics, with special emphasis on the interaction between experimental and theoretical physical chemistry, chemical physics, materials and life sciences.

ISTCP-2024

Conference theme

Theoretical algorithm software of theoretical chemistry physics and its application

- ◎ Electronic and nuclear dynamics & statistics (ENDS)
- ◎ Wave function theory for electronic structure (WFT)
- ◎ Density functional theory and time-dependent density functional theory for electronic structure (DFT)
- ◎ Low-order scaling methods for electronic structure (O(N))
- ◎ Quantum computing for quantum chemistry (QC4QC)
- ◎ Computational spectroscopy (SPECT)
- ◎ Computational catalysis (CAT)
- ◎ Computational biology (BIO)
- ◎ Computational materials (MATER)
- ◎ Machine learning and data-driven approaches (MLDD)
- ◎ Embedding methods for electronic structure (EMBED)
- ◎ Software design and development (SOFT)
- ◎ Relativistic electronic structure theory of heavy-element chemistry (Relativity)
- ◎ Auqing Tang, Joe Paldus, and Bogumil Jeziorski memorial symposium/Chemical insights (MEM)

Host

International Society of Theoretical Chemical Physics
Shandong University

Organizer

School of Chemistry and Chemical Engineering, Shandong University

Chair: Wenjian Liu
Vice chair: Erkki Brändas

International Advisory Committee

Gustavo Aucar, Ria Broer, Hazel Cox, Jürgen Gauss, Peter Gill, Leticia González, Kersti Hermansson, Mark R. Hoffman, Chao-Ping Hsu, Jin Yong Lee, Shuhua Li, Eduardo Ludena, Benedetta Mennucci, Hiromi Nakai, Jozef Noga, Sourav Pal, Martin Quack, Dennis Salahub, Peter Schwerdtfeger, Thereza A. Soares, Péter R. Surján, Alja Tadjer, Oscar Ventur

Local Organizing Committee

Wenjian Liu, Yuxiang Bu, Yang Guo, Zhonghan Hu, Jilai Li, Haibo Ma, Yuchen Ma, Dongju Zhang, Hao Wang, Qiunan Xu, Chenyu Wu, Xiaoyu Xie

Contacts

Fan Li: +86 13325025598
Qian Wang: +86 17865429321
Email: istcp@istcp2024.com

General Information

Conference time

13-18 October, 2024

Opening hours of the registration desk

Saturday, 12 October, 2024	14:00-18:30
Sunday, 13 October, 2024	08:30-17:00
Monday, 14 October, 2024	08:30-17:00
Tuesday, 15 October, 2024	08:30-17:00
Wednesday, 16 October, 2024	08:30-17:00
Thursday, 17 October, 2024	08:30-17:00

Name Badges

During the congress, please wear your badge at all times. The badge is your entrance ticket to the session halls.

Lectures

The length of the talks is as follows:
Plenary Lectures: 37 min talk + 8 min discussion
Invited Lectures: 25 min talk + 5 min discussion

Poster Awards

The winners will be announced during the closing ceremony on Friday, 18 October. Attention: The winners of the poster awards need to attend the closing ceremony. If a winner is absent at the ceremony, the award will be awarded to the next candidate on the list.

Floor Plan

【Registration】 Huanghai Hotel Lobby (黄海饭店大堂)

【Opening & Closing】 Room 1 & 2, first floor (二楼会议中心)

【Plenary Lectures】 Room 1 & 2, first floor (二楼会议中心)

【Parallel Sessions】 There are 6 parallel sessions as below.

① Room 1, first floor (二楼会议中心前区)

② Room 2, first floor (二楼会议中心后区)

③ Room 3, first floor (二楼会议厅)

④ Room 4, second floor (三楼第二会议室)

⑤ Room 5, third floor (4 楼锦绣厅)

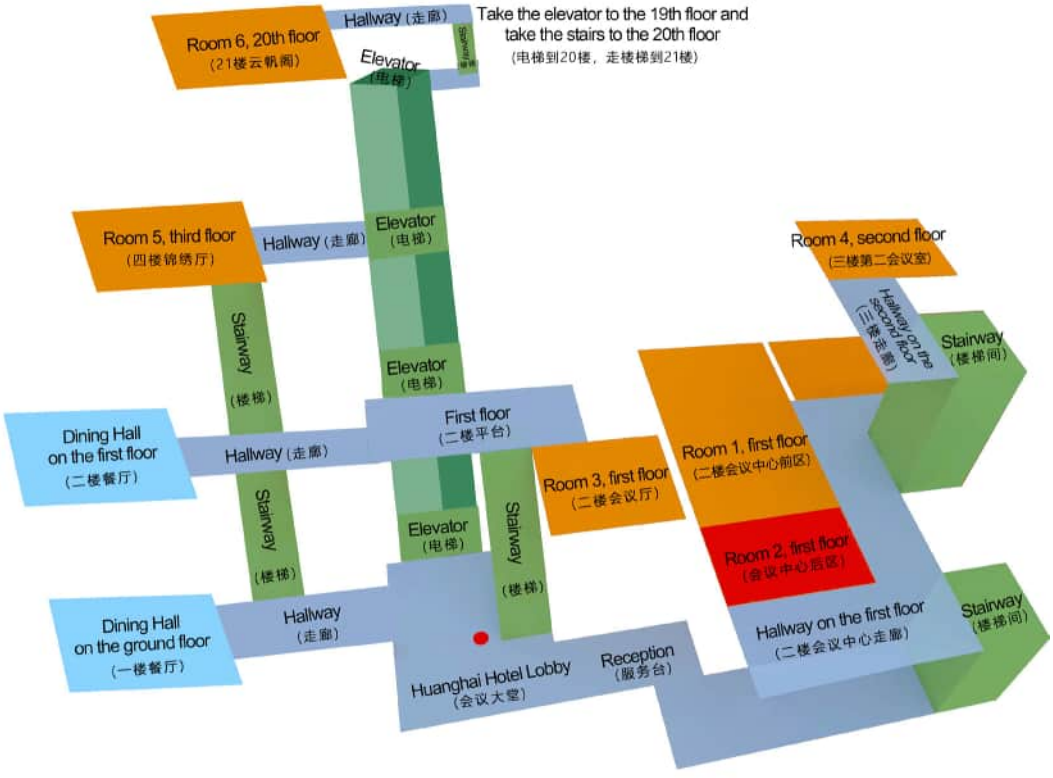
⑥ Room 6, 20th floor (21 楼云帆阁)

【Poster】 Hallway on the first floor (二楼会议中心走廊)

【Welcome Reception】 Dining Hall on the ground and first floor

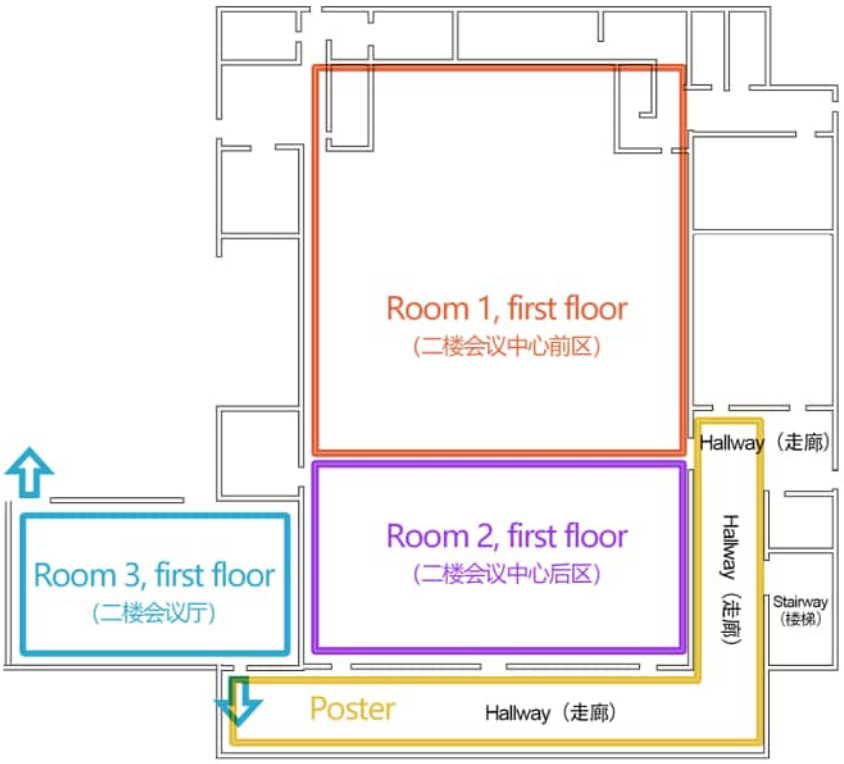
【Lunch】 Dining Hall on the ground and first floor

【Conference Dinner】 Room 1 & 2, first floor (二楼会议中心)



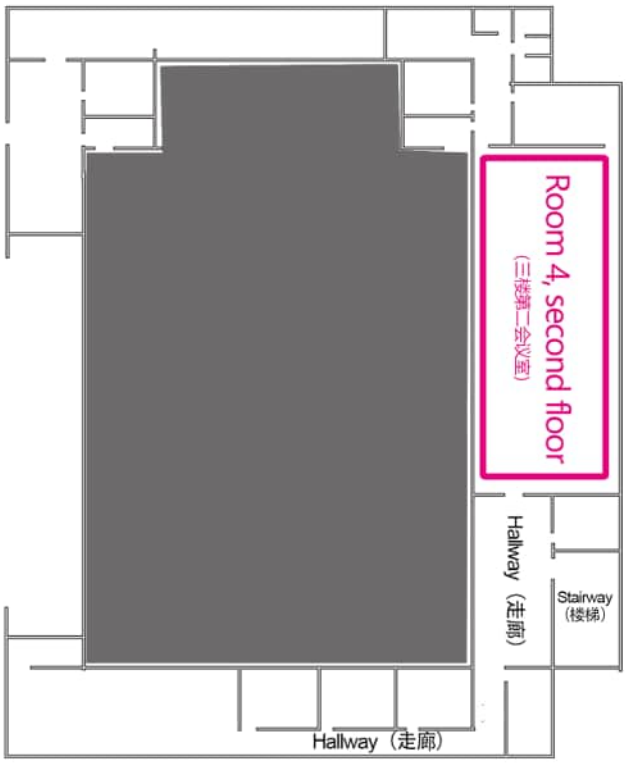
Conference Rooms on the first floor

（黄海饭店二楼会议室）



Conference Rooms on the second floor

（黄海饭店三楼会议室）



MattVerse Limited

Mission

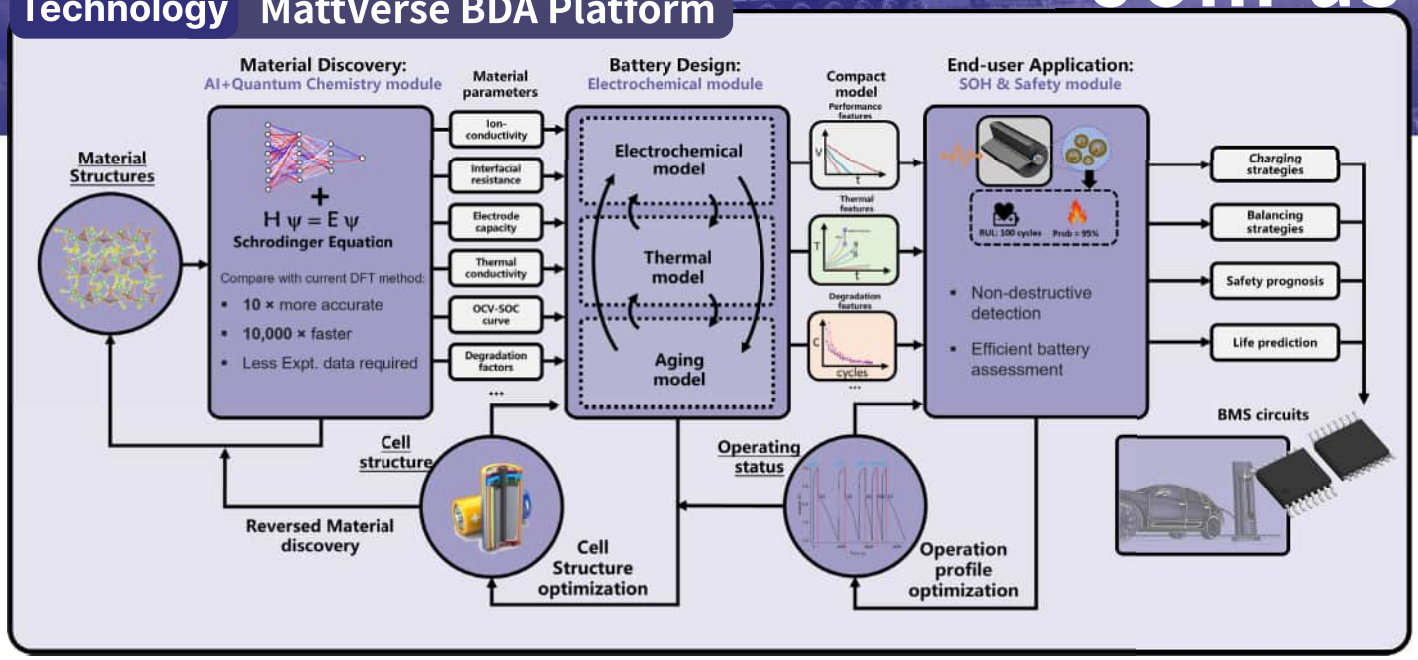
Develop and commercialize **Battery Design Automation (BDA)** for new energy industry

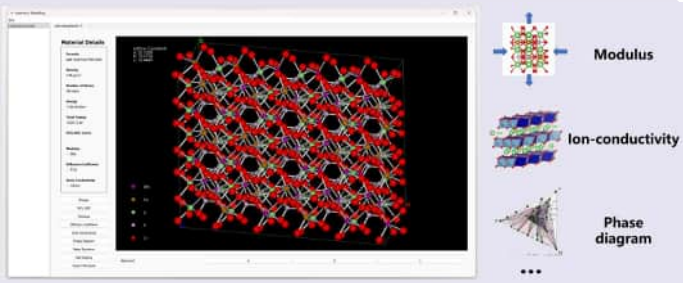
Vision

Combining AI and multiscale simulation, we strive to **accelerate the development of new energy industries.**

Join us!

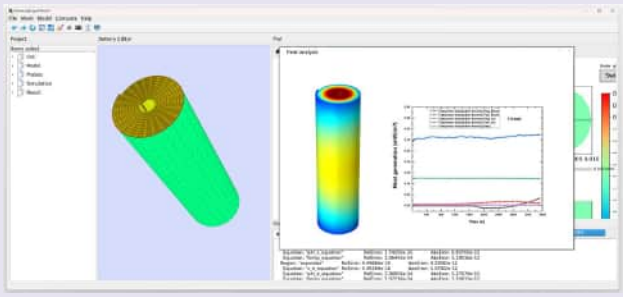
Technology MattVerse BDA Platform





The combination of AI and quantum chemistry methods leads to material property predictions that are 1 order of magnitude more accurate and 4 orders of magnitude faster than traditional methods.

Material Discovery

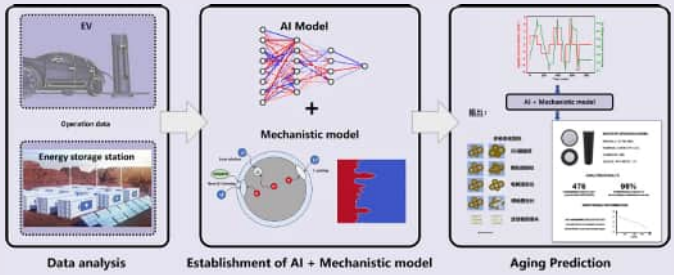


Cell Design

By leveraging AI and smart mesh generation technologies, the efficiency of battery simulation is increased by 2 orders of magnitude. With intrinsic material properties included, dynamic and accurate predictions of battery aging processes are achieved.

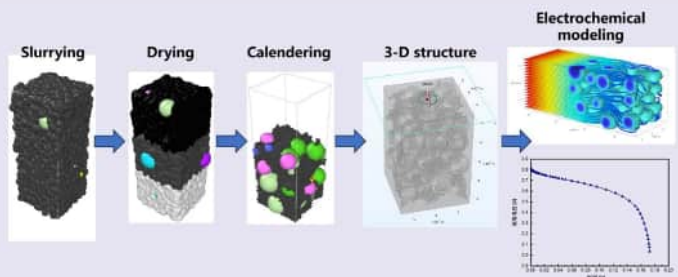
Through a unique AI + mechanistic model, it is possible to extract multidimensional aging information, such as lithium dendrite growth, from short-term charging and discharging data. This enables accurate predictions of the battery's remaining useful life and thermal runaway risk.

BMS Application



Process optimization

Using advanced kinetic simulation technology, the effects of manufacturing processes such as slurry mixing, drying, and calendering on the mesoscopic morphology of electrodes and battery cell performance are evaluated, thereby bridging the gap between material development and battery cell design.



MattVerse Limited Unit 915 of 17W Building, Science Park, NT, Hong Kong Email: info@mattverse.com

ByteDance Research

About Us

ByteDance Research focuses on frontier technologies in the field of AI, including AI for Science, Machine Translation, Video Foundation Model, Robotics Research, Machine Learning Fairness, etc. At the same time, it is committed to applying research findings, providing technical support and services for the company's existing products and businesses.

Our AI for Science team is dedicated to addressing challenges in biology, physics, and materials science through advanced computational tools, including Machine Learning, Computational Chemistry, and High-Throughput Computation. Our aim is to drive breakthroughs in natural sciences with innovative methodologies, ultimately contributing to global progress and well-being.

Research Fields

Quantum Chemistry and Machine Learning Force Field

In this interdisciplinary field of quantum chemistry and machine learning force fields, we merge deep domain knowledge in physics and chemistry with fast-paced, data-driven research and engineering. Our focus is on the contributions to GPU-accelerated density functional quantum chemistry software, GPU4PySCF, which is open-sourced to facilitate fast and high-quality data curation. Leveraging this robust data foundation, we advance state-of-the-art machine learning force fields and molecular dynamics technologies to address critical challenges in biology and materials science.

Machine Learning for Biology and Chemistry

We focus on scaling up models, data, and applicable systems with general representation and architecture, aiming to tackle scientific challenges previously considered insurmountable. Our focus areas include:

- Build models for various biological molecules involving proteins, nucleic acids, and organic small molecules to solve problems related to structure/conformation prediction, property prediction, and molecule generation.
- Combining large language models and multimodal capabilities to address practical challenges in the fields of biology and chemistry.

Neural Network based Quantum Monte Carlo

We focus on developing neural network-based Quantum Monte Carlo methods that leverage the powerful expressiveness of neural networks to directly represent wavefunctions. This approach provides high accuracy and the capability to handle strongly correlated and multi-reference systems. Through our innovative research, we are pioneering advancements in this emerging field.

Large Scale Ab initio Quantum many body Calculation

We are dedicated to enhancing quantum chemistry simulations for large-scale systems, crucial for a wide range of applications including chemical reactions, catalysis, superconductivity, and surface chemistry. We focus on developing and applying various quantum embedding methods to systems up to 100,000 orbitals, especially those with significant electron correlations. Leveraging modern quantum chemistry approaches, such as quantum algorithms and quantum Monte Carlo methods, we aim to create advanced, accurate simulation tools.

Selected Research Papers

- BAMBOO: a predictive and transferable machine learning force field framework for liquid electrolyte development
  Arxiv
- Enhancing GPU-acceleration in the Python-based Simulations of Chemistry Framework
  Arxiv
- GPU-Accelerated AFQMC
  Arxiv
- Symmetry enforced solution of the many-body Schrödinger equation with deep neural network
  Nature Computational Science in press
- A computational framework for neural network-based variational Monte Carlo with Forward Laplacian
  Nature Machine Intelligence 6.2 (2024): 209-219.
- Electric Polarization from a Many-Body Neural Network Ansatz
  Physical Review Letters 132.17 (2024): 176401.
- Towards the ground state of molecules via diffusion Monte Carlo on neural networks
  Nature Communications 14.1 (2023): 1860.
- Ab initio calculation of real solids via neural network ansatz
  Nature Communications 13.1 (2022): 7895.
- Toward practical quantum embedding simulation of realistic chemical systems on near-term quantum computers
  Chemical Science 13 (31), 8953-8962
- Ab initio quantum simulation of strongly correlated materials with quantum embedding
  npj Computational Materials 9 (1), 78

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标准化

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- 面向高校、科研院所和企业的研发用户
- 服务于医疗、化工、半导体等多个行业的科研领域

解决方案

- 机器化学家平台设计
- 设备个性化定制
- 设备适配增值改造
- 平台升级服务
- 无人智慧实验室建设

应用效果

- 增效降本、精准智造
- 面向需求逆向创制新物质
- 赋能合成机器人自适应优化、功能材料逆向设计、生物医学精准控制等

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