The 7th China-Japan-Korea Workshop on Theoretical and Computational Chemistry

Hosted by:

College of Chemistry and Chemical Engineering, Xiamen University

State Key Laboratory of Physical Chemistry of Solid Surfaces

Fujian Key Laboratory of Theoretical and Computational Chemistry

November 24-27, 2025

Xiamen, China

TABLE OF CONTENTS

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SPONSORS

This workshop is sponsored by Dawning Information Industry (Beiiing) Co., Ltd.

VENUE

Hotel: Yifu Building

Registration: Lobby of Yifu Building

Meeting: Room 202, Lujiaxi Building

Poster: Lobby of Lujiaxi Building

Lunch: Ea Cafe

Dinner: Linwutong Building

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SCIENTIFIC PROGRAM

Monday, November 24, 2025	
14:30-19:00	Registration
Tuesday, November 25, 2025	
08:45-09:00	Opening Remark & Photo
Session I	**Chair: Wei Wu**
09:00-09:50	**Neil Qiang Su (China)** Hierarchically Correlated Orbital Functional theory: Theory, Algorithms, and Functionals
09:50-10:40	**Min-Cheol Kim (Korea)** Density Functional Theory for Catalysis and Electrocatalysis
10:40-11:00	Tea Break
Session II	**Chair: Hiromi Nakai**
11:00-11:50	**Chen Li (China)** Localized Orbital Scaling Correction to Linear-response Time-dependent Density Functional Approximations
11:50-12:40	**Airi Kawasaki (Japan)** Geminal-Based Wavefunctions for Strongly Correlated Electron Systems
12:40-13:30	Lunch BOX
Session III	**Chair: Jin Yong Lee**
13:30-14:20	**Hyungjun Kim (Korea)** Quantum Interference in Singlet Exciton Fission
14:20-15:10	**Jaehoon Jung (Korea)** Enolate as A Key Ingredient in the Formation of Highly Ordered OH-functionalized Graphene
15:10-16:00	Tea Break & Poster Session
Session IV	**Chair: Shuhua Li**
16:00-16:50	**Masato Kobayashi (Japan)** Tackling Strong Electron Correlation via Divide-and-conquer Approaches
16:50-17:40	**Wei Li (China)** Accurate Treatment of Large and Strongly Correlated Systems: From

	Fragmentation Approaches to Block-Correlated Coupled-Cluster Theory
17:40-18:30	**Chinami Takashima (Japan)** Divide-and-Conquer Method Using Two-particle Reduced Density Matrix to Incorporate Static Corrlation
18:30-20:00	Dinner
	Wednesday, November 26, 2025
Session V	**Chair: Yi Zhao**
08:45-09:35	**Jiajun Ren (China)** Quantum Dynamcs Algorithms for Electron-Vibration Coupled Systems: Tensor Network and Quantum Computing
09:35-10:25	**Yasuhiro Ikabata (Japan)** Theoretical Investigation for Understanding Electronic Structure of Minimum Energy Conical Intersection
10:25-10:45	Tea Break
Session VI	**Chair: Wanzhen Liang**
10:45-11:35	**Seunghoon Lee (Korea)** Simulating X-ray Spectra of Transition-Metal Sulfide Systems
11:35-12:25	**Dong Yeon Kim (Korea)** Interdisciplinary Applications of Computational Chemistry in Materials Science
12:25-13:30	Lunch BOX
	Thursday, November 27, 2025
Session VII	**Chair: Wenjian Liu**
08:45-09:35	**Enhua Xu (Japan)** Tensor-product Bitstring Selected Configuration Interaction
09:35-10:25	**Chen Zhou (China)** Valence Bond Theory for Strongly correlated Systems
10:25-10:45	Close Remark

POSTER PROGRAM

P-01	Shengyang Cai	Unraveling the Catalytic Mechanism and Substrate Selectivity of HDAC10: A Dual-Filter Approach for Polyamine Deacetylation
P-02	Jinji Cao	New Insights into Li^+/Mg^{2+} Separation by A CNT Model Membrane via Coupling High-throughput Simulations and Machine Learning
P-03	Yuxinxin Chen	UAIQM – the Ultimate Solution to the Universal AI Models for Atomistic Simulations beyond DFT
P-04	Siyuan Gao	Phonon-Mediated Ultrafast Energy- and Momentum- Resolved Hole Dynamics in Monolayer Black Phosphorus
P-05	Guoyan Ge	Theoretical Simulations of Steady-State and Time-Resolved X-Ray Absorption Spectroscopy for Complex Systems
P-06	Qiuyue Ge	Exciton Dynamics in Edge-on ZnPc–F8ZnPc System: Insights from Quantum Simulations
P-07	Fanhong Han	Multireference Block-Correlated Coupled Cluster Theory with up to Five-pair Correlation
P-08	Takuya Hashimoto	Development of Gaussian Charge Distributed Harmonic Solvation Model
P-09	Jinming Hu	Aitomia: AI Agents for Autonomous AI-Driven Atomistic Simulations
P-10	Jingxin Hu	Construction of fused BN-heterocycles *via* boron atom insertion: DFT insights into the Lewis acid–base (BBr_3/NEt_3) cooperative mechanism and selectivity
P-11	Xunkun Huang	Time-Dependent Kohn−Sham Electron Dynamics Coupled with Nonequilibrium Plasmonic Response via Atomistic Electromagnetic Model
P-12	Ryuto Kambara	Theoretical Study on Dynamically Hidden Reaction Path: Dissociation of C^+ from Doubly Ionized OCS
P-13	Baotao Kang	Revealing Common Nature of O And S Doping in Enhancing the Oxygen Electrocatalytic Performance of FeN4
P-14	Zhihao Lan	Variational Quantum Simulation of Time-Local Quantum Master Equations via Quantum Jump

P-15	Nannan Li	MXenes Enhance Electrocatalytic Water Electrolysis of NiFe Layered Double Hydroxides through Bifunctional Heterostructuring
P-16	Xiaoyuan Liu	Multi-Scale Mechanisms Reveal the Synergistic Strategy of Remote Mutations in MPH Enzyme for Enhancing Stability and Activity
P-17	Tairen Long	Rational Design of Transition Metal–Phosphorus Dual-Atom Catalysts in Defective h-BN for CO_2 Hydrogenation and Cycloaddition
P-18	Xingyuan Lu	PyMEDA: A Unified Python Framework for Multiscale Energy Decomposition Analysis
P-19	Ruitong Ma	A Theoretical Study on the Mechanism of Strain-Regulated Oxygen Evolution Reaction Performance of RuO_2
P-20	Gen Ogawa	Divide-and-Conquer MP2 for Periodic Systems
P-21	Rei Oshima	Unitary Matrix Optimization in Quantum Chemistry with Givens Rotation and Error Backpropagation
P-22	Cheng Peng	Theoretical Insights into Exchange Coupling Interactions in Two Biomimetic Mixed-Valence Manganese Complexes: A DMRG Study
P-23	Xinyu Sun	Efficient Evaluation of Spin-Orbit Couplings in Single-Molecule Magnets Using DMRG within the DMET Framework
P-24	Yingqi Tang	Insights into Proton Transfer Dynamics in Histidine Tautomers of Amyloid-β (1-40)
P-25	Xinyu Tong	Theoretical Study of Linearly Fused Imide-functionalized Thienoacenes and Universal Machine Learning Potentials for Excited States
P-26	Xuerong Wang	A Template-Based Automatic Fragmentation Algorithm for Generalized Energy-Based Fragmentation Approach
P-27	Xun Wu	Development of High-Accuracy Diabatization Methods Based on Valence Bond Theory
P-28	Dongxu Xie	Theoretical Study on Graphdiyne-Supported Cyclo[16/18] Carbon for Application in Lithium-Ion Batteries
P-29	Yuchuan Xu	Electronic Absorption and Circular Dichroism Spectra of One-Dimensional Bay-Substituted Chiral PDIs: Effects of Intermolecular

		Interactions, Vibronic Coupling, and Aggregate Size
P-30	Jun Yu	Rationally Computational Engineering Diisopropyl Fluorophosphatase for Novichok A234 Detoxification
P-31	Suxin Yu	A Deep Learning-Based Framework for Valence Bond Structure Selection and Weight Prediction
P-32	Yabing Zeng	Triplet-Triplet Conversion Mediated by Spin-Orbit Coupling: A Diabatic Perspective of $Ru(bpy)_3^{2+}$
P-33	Huizhu Zhang	Adiabatic-to-Diabatic Analysis Method for Multi-State Systems
P-34	Miaorun Zhang	AuI Complexes with Planar Tetracoordinate Carbon and Their Catalytic Activity for the Rearrangement of Allylic Acetates: A Computational Study
P-35	Yueyang Zhang	Intermolecular Dispersion Interactions: Low-Rank Algorithms and Energy Decomposition
P-36	Hangjing Zheng	Effective Two-State Model Based on Adiabatic-to-Diabatic Transformation and Its Applications
P-37	Jingxiang Zou	MOKIT: An Open-Source Framework for Interoperability Among Quantum Chemistry Packages

Formulation and Advancement of Hierarchically Correlated Orbital Functional Theory

Neil Qiang Su (苏乃强)

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Kohn-Sham Density Functional Theory (KS-DFT) and Reduced Density Matrix Functional Theory (RDMFT) provide two distinct yet rigorous frameworks for addressing many-electron problems. However, both approaches face intrinsic challenges in describing static and dynamic correlation effects. In light of this, we have developed the Hierarchically Correlated Orbital Functional Theory (HCOFT), which unifies KS-DFT and RDMFT within a single theoretical framework, offering new avenues for improving the accuracy of electronic-structure predictions. This presentation will summarize recent progress in our group on the theoretical foundations, computational algorithms, and approximate functionals developed along this direction.

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Education

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• 2009 B.Sc., Xiamen University

Professional Career

• 2020-Now Professor, Nankai University

• 2016-2020 Postdoctoral researcher, Duke University

• 2015-2016 research assistant, Fudan University

Research Interests

Development of functional theories for electronic structure, including Kohn-Sham density functional theory (KS-DFT), reduced density matrix functional theory (RDMFT), and the Hierarchically Correlated Orbital Functional Theory (HCOFT) proposed by his group.

Density Functional Theory for Catalysis and Electrocatalysis

Min-Cheol Kim

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Nowadays, the global environmental crisis including fossil fuel depletion and global warming has become a severe problem. To overcome these issues, renewable and green energy sources are of great interest, and hydrogen energy is one of the most promising methods to achieve green energy. The hydrogen industry consists of various important processes related to hydrogen, including fuel cells, hydrogen production, and conversion. These processes involve chemical reactions from one chemical substance to another chemical substance, and these reactions can be accelerated with (electro)catalysts. Therefore, designing novel catalysts and electrocatalysts is essential to realize a true renewable and green energy process.

In silico materials design is a powerful and practical tool for designing novel materials using quantum chemical simulations such as the density functional theory (DFT), which can significantly reduce the cost than trial-and-error bases experimental approaches and enables rational design of energy materials. In this presentation, I introduce how to utilize quantum chemical simulations techniques to provide novel design strategies for hydrogen production catalysts and ammonia-mediated hydrogen conversion catalysts.

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- 2015 - 2017 Postdoctoral researcher, Theoretical and Computational Chemistry Lab, Yonsei University

Research Interests

In Silico Design of Electrochemical catalysts and Energy Materials; development of Quantum Chemistry Methods for Electrochemistry

Density Functional Approximations Guided by Exact Constraints

Chen Li

College of Chemistry and Molecular Engineering, Peking University

The present-day commonly used density functional approximations (DFAs) suffer from various systematic errors, and they can all be attributed to the violation of some exact constraints. In the first part of my talk, I will focus on two important constraints: (i) the Perdew-Parr-Levy-Balduz (PPLB) linearity condition for fractionally charged systems; and (ii) proper energy behavior in the semi-classical limit $\hbar \to 0$. Guided by the first constraint, we have developed the localized orbital scaling correction (LOSC) functional that restores the PPLB condition through specially designed localized orbitals, called orbitalets. The LOSC functional can largely improve molecular dissociation problems, HOMO-LUMO gaps and photoemission spectra. Our recent development of combining LOSC with linear response TDDFT has greatly improved excitation energies, particularly for Rydberg and charge-transfer excitations. The second constraint is highly relevant to strongly correlated systems. Through a model atomic calculation, we show that the exact total energy as $\hbar \to 0$ saturates to a finite value, whereas the mainstream DFAs have qualitatively wrong divergent behavior of $\hbar^{-1/6}$. By introducing an effective $\hbar$ for valence electrons, we estimate that the $\hbar$eff for such systems can be as small as 0.2. Thus, this exact constraint might inspire novel functional approximations for describing strong correlation. In the second part of my talk, I will discuss our recently developed method for solving Schrödinger equations, which allows us to obtain the exact analytic structure of wave functions for one and two-body problems, and can be further generalized to many-body problems. The analytic expression of the ground state wave function is ultimately cast into an exact factorized form including a pre-exponential power factor, an exponential decaying term and a modulator, a mildly-varying and bounded function that can be easily approximated. This novel analytic structure serves as a new starting point for developing approximations that go beyond the single electron picture.

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Education

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Professional Career

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- 2019.10 – 2020.08 Postdoctoral researcher, Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Israel
- 2017.04 – 2019.08 Postdoctoral researcher, Max Planck Institute of Microstructure Physics, Germany
- 2016.12 – 2017.03 Postdoctoral researcher Postdoctoral researcher, Duke University, USA

Research Interests

Li Group is engaged in developing density functional theory methods, aiming at predicting chemical reactions with a high precision, describing reaction mechanisms, and predicting properties of small molecules, big molecules and solid state materials. With our theory, we hope to explain, predict and ultimately guide the experiment. Regarding applications, our present focuses are: reaction mechanisms of catalytic processes, and chemical evolution processes after photo-excitation. Our research projects include:

1. Starting from the LOSC functional, improving the functional approximation for correcting molecular dissociation problems near the equilibrium.
2. Extending the LOSC functional form from finite to extended systems, in order to predict material properties of solid states.
3. Developing beyond Born-Oppenheimer time-dependent density functional methods and

explicitly bringing the nuclear motion into the framework of density functional theory, for simulating nonadiabatic chemical reactions, such as chemical evolution processes after photo-excitation.

4. Solving exactly dissociation problems of diatomic molecules, and bringing new insight into the design of novel density functionals.

Geminal-Based Wavefunctions for Strongly Correlated Electron Systems

Airi Kawasaki

Gunma University

Division of Electronics and Mechanical Engineering, Graduate School of Science and Technology

I. Introduction

To calculate strongly correlated systems accurately, one needs to treat strong and weak correlations simultaneously. Hartree-Fock (HF) theory and density-functional theory are able to deal with the weak correlation, but not with the strong correlation. On the other hand, the full-CI method provides the exact solution including both the weak and strong correlations, though it needs huge computational cost. In this context, we focused on electron pair wave-function theory. In the field of chemistry, the concept of electron pair has been used to represent a chemical bond for a long time.

The electron pair is called a geminal in chemistry and many calculation methods using geminals have been developed.

II. Method

In this study, we focused on the antisymmetric product of geminals (APG) wavefunction, which expresses each electron pair using a different geminal matrix. We solved the variational complexity of the APG wavefunction by using the polynomial decomposition and applied the APG wavefunction to the Hubbard model and the water molecule. To explore the nature of electron correlation in the geminal wavefunction, we analyzed the eigenvalues of the geminal antisymmetric matrices in the obtained APG wavefunction. As a result, we clarified that only N/2 or fewer eigenvalues have non-zero values in the N-electron system. Therefore, we developed a theory with high accuracy and low cost by reconstructing the wavefunction using only the important eigenvalues. This corresponds to lowering the rank of the geminal matrix.

The optimization of the low-rank APG wavefunction is performed by alternately optimizing the eigenvalue part and the orbital part represented by unitary matrices. During the optimization of the orbital part, the unitarity condition must be strictly preserved. In this work, we employ

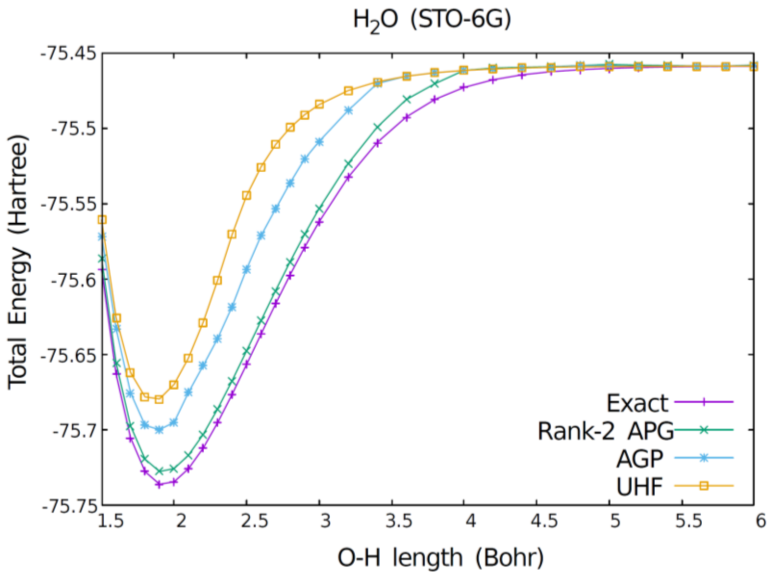
Givens rotation matrices to represent the unitary matrix and incorporate them into the direct Givens rotation (DGR) framework, achieving an efficient and stable optimization process.

III. Results

We applied the low-rank APG methods to the Hubbard model, H_2O and N_2. As a result, the low- rank APG method achieved higher accuracy than the antisymmetrized geminal power (AGP) and HF even at rank-2, successfully capturing the potential energy curves of both H_2O and N_2.

Furthermore, we analyzed the wavefunction by calculating the density matrix and double occupancy while changing the value of Hubbard U, and discussed how the low-rank APG expresses the correlation.

The low-rank APG is a flexible method that allows tuning of the included electron correlation by varying the rank. Moreover, even at the same rank, it can represent a variety of wavefunction forms, providing additional flexibility. Therefore, the low-rank APG method is expected to serve as a highly accurate and computationally efficient approach applicable to a wide range of strongly correlated electron systems.



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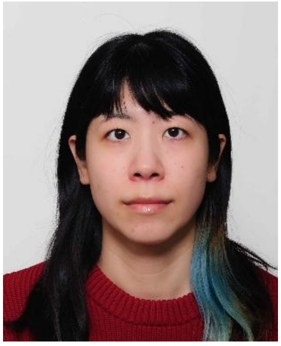
Airi Kawasaki



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Research Interests

- Wave function theory
- Strongly correlated system
- Geminal theory
- Embedding theory
- Tensor decomposition
- Quantum theory of atoms in molecules

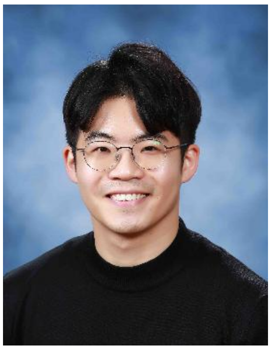
Diverse Quantum Interference Regime in Intramolecular Singlet Fission Chromophores

Hyungjun Kim

Hanyang University

An array of heterocyclic π-conjugated linkers, thiophene derivatives, in covalently linked pentacene dimers illustrates how quantum interference (QI) modulates nonadiabatic coupling (NAC) during the multiexciton formation (MEF) step in singlet fission (SF). Subtle structural isomerism—particularly in sulfur orientation—alters NAC significantly, despite minimal energetic changes. Extended curly arrow rules classify the resulting QI regimes (constructive, destructive, and shifted destructive), and nonequilibrium Green's function calculations with density functional theory corroborate these findings. Notably, the degree of charge resonance and appearance of charge-transfer excitations both hinge on the operative QI regime, captured effectively by NAC magnitude. Further, we investigated the impact of nitrogen doping at the benzene linkers on the QI behavior. Overall, these insights underscore the critical role of QI in dictating MEF dynamics, offering a clearer structure–property framework for tailoring intramolecular SF systems.

Hyungjun Kim



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Research Interests

- Understanding electronically excited state dynamics in singlet fission
- Theory development to improve electron dynamic correlation description in spin-flip RAS framework
- Application of molecular dynamics for describing polymer behavior

Enolate as A Key Ingredient in the Formation of Highly Ordered OH-Functionalized Graphene

Jaehoon Jung

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The molecular behaviors, such as adsorption, diffusion, desorption, and chemical reactions, and their uniform arrangements on solid surfaces are important research topic, not only as fundamental subjects in surface science but also for applications in heterogeneous catalysis, sensing, and molecular-scale electronic devices. The interfacial interaction between molecules and substrates has long served as a key factor in achieving robust predictability and high controllability in a variety of applications. Herein, recent computational investigations based on density functional theory (DFT), conducted in close conjunction with scanning tunneling microscopy (STM) experiment at atomic spatial resolution, provide insights into: (i) selective molecular diffusion controlled by electric fields on ultrathin insulating films and (ii) the role of enolate in the formation of highly periodic two-dimensional graphenol structures.

In this study, DFT calculations revealed that graphene enolate plays a crucial role in forming the $C_6(OH)_1$ superstructure on Cu(111).[1] The enolate forms via a barrierless reaction between hydroxyl groups and promotes low-barrier diffusion, guiding the assembly of ordered OH patterns. It also stabilizes intermediate water molecules, facilitating the formation of double-meta OH configurations. This pathway is energetically favored over the formation of $C_6(OH)_2$, consistent with the dominant experimental observation of $C_6(OH)_1$.

Furthermore, several research projects will be briefly introduced to share the current activities of our laboratory.

Reference

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Professional Career

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Tackling Strong Electron Correlation via Divide-and-Conquer Approaches

Masato Kobayashi

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We have developed divide-and-conquer (DC) linear-scaling electronic structure methods, particularly for mean-field (i.e., HF/DFT) and dynamical electron correlation theories [1]. However, describing strong (or static) electron correlation in large systems based on the fragmentation approach remains challenging. This presentation introduces our recent attempts to tackle strong electron correlation via the DC method.

I. DC Hartree–Fock–Bogoliubov (HFB) method

The HFB method, originally developed as a mean-field theory for Bogoliubov quasiparticles and applied to electronic structure in Ref. [2], is related to the geminal-based wavefunction, which can describe the static electron correlation. We have proposed the DC-HFB method as an efficient static correlation theory for large systems [3]. Recently, we have derived the gradient of the DC-HFB energy and applied it to the geometry optimization of graphene nanoribbon systems [4].

II. DC projected unrestricted Hartree–Fock (PUHF) method

Although unrestricted HF (UHF) energy can also be used to approximate the static electron correlation, the UHF and HFB wavefunctions suffer from spin and electron-number contamination, respectively. Applying the projection operator to these wavefunctions can extract the desired quantum-number state [5]. We are currently developing a DC-based projected UHF method.

III. DC electron correlation calculation on quantum computer

The variational quantum eigensolver (VQE) is a widely used method for quantum chemical computations on quantum computers. Yoshikawa *et al.* [6] proposed the DC-VQE method to reduce the number of qubits and quantum gates required for large systems. In collaboration with Prof. Yoshikawa, we examined the practical performance of the DC-VQE method on the non-error-tolerant quantum devices.

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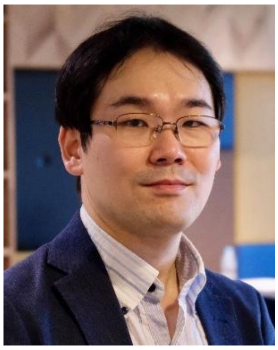
Masato Kobayashi



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Research Interests

• Electronic structure theory
• Theoretical Chemistry
• Quantum Chemistry
• Quantum Chemical Informatics
• Linear-scaling quantum chemical methodologies
• Electron correlation theory

Accurate Treatment of Large and Strongly Correlated Systems: From Fragmentation Approaches to Block-Correlated Coupled-Cluster Theory

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Accurate quantum chemistry treatments of large and strongly correlated systems remain highly demanding due to the steep scaling and limited applicability of conventional single-reference methods. To overcome these challenges, we have developed two categories of theoretical frameworks: energy- and localized molecular orbital (LMO)-based fragmentation approaches for large systems, and block-correlated coupled-cluster (BCCC) theories for strongly correlated electronic structures. The generalized energy-based fragmentation (GEBF) and cluster-in-molecule (CIM) approaches reconstruct energy and energy derivatives from electrostatically embedded subsystems or LMO clusters, enabling high-level electronic correlation calculations of macromolecules and condensed-phase systems. Recent progress includes GEBF geometry optimizations and vibrational spectra calculations of large molecular crystals,[1] automated SMILES-encoded template-based GEBF approach,[2] analytical gradients for CIM-RI-MP2,[3] reduced CIM strategy for host-guest interactions,[4] and etc. In parallel, the generalized valence bond–based BCCC (GVB-BCCC) hierarchy provides a scalable multireference framework for capturing static correlation of strong correlated systems. Newly implemented GVB-BCCC3–5 methods systematically extend electron-pair correlations, yielding accurate ground-state spin multiplicities[5] and static correlation energies consistent with benchmark multireference results.[6-7]

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Research Interests

- Linear-scaling electronic structure methods
- strongly correlated quantum chemistry
- machine-learning force fields
- software development

Divide-and-Conquer Method Using Two-Particle Reduced Density Matrix to Incorporate Static Correlation

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Large-scale calculations of correlated systems remain a major challenge in quantum chemistry. The divide-and-conquer (DC) method[1] is one of the fragmentation schemes for large systems by treating the entire system as a sum of subsystem contributions. The DC methods are typically categorized into two types: density-matrix-based and energy-based schemes[2]. The former constructs a total density matrix from the subsystem density matrices to calculate total energy, thereby accurately accounting for both short- and long-range interactions. The DC-based Hartree–Fock (HF) method[3] succeeded in describing HF exchange interaction that has long-range behaviors, by constructing the total Fock matrix from the total density matrix assembled from subsystem contributions. The latter evaluates total energy from subsystem contributions, mainly incorporating short-range interactions. The conventional DC-correlation methods[4–6] are energy-based schemes; thus they struggle to describe static correlation that mainly involves long-range effects.

The aim of this study is to develop a DC-correlation method that effectively incorporates static correlation. In this presentation, we propose a hybrid DC-correlation method that combines the density-matrix- and energy-based DC schemes utilizing the characteristics of two-particle reduced density matrix[7]. In this method, the electronic energy is decomposed into terms represented by one-particle reduced density matrix and two-particle cumulant. The extensivity of the two-particle cumulant[8] is exploited. Numerical assessments showed that the present method well reproduces the full configuration interaction results in the description of stretched hydrogen chains that are affected by long-range static correlation. The results suggest the validity of the hybrid DC-correlation method for describing long-range, i.e., static correlations.

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Research Interests

Development of large-scale calculation methods in electronic structure theory. Two-component relativistic theory. Electron correlation methods.

Tensor Network Algorithms for Electron-Vibration Coupled Dynamics

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Understanding the real-time dynamics and dynamical properties of electron–vibration coupled systems is essential for elucidating fundamental processes such as energy transfer, separation, and relaxation in molecular and condensed-phase systems. However, exact quantum dynamics simulations are severely limited by the exponential growth of computational cost with system size. In this talk, I will present our recent developments of tensor network algorithms for accurately and efficiently simulating electron–vibration coupled dynamics. We developed efficient time-dependent density matrix renormalization group (TD-DMRG) algorithms within the matrix product state and matrix product operator framework, enabling numerically exact quantum dynamics with polynomial computational scaling.[1-2] For condensed-phase systems, we have proposed an improved memory truncation scheme via influence functional renormalization that enhances the accuracy of real-time path-integral calculations.[3] These methods are applied to study the effects of excitonic coupling on nonradiative decay rate of molecular aggregates, revealing non-monotonic behaviors of decay rates with energy gaps.[4-5]

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Research Interests

Development of high-accuracy quantum dynamics methods based on tensor network states and the theoretical investigation of excited-state dynamics in complex molecular systems.

Theoretical Investigation for Understanding Electronic Structure of Minimum Energy Conical Intersection

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Conical intersections (CIs) are essential for radiationless deactivation from electronically excited states. Quantum chemical calculations have been performed to obtain the geometries of minimum energy CIs (MECIs). The interpretation and prediction of MECI geometries are difficult compared to equilibrium geometries. We have discovered relationships related to the electronic structure at the S_0/S_1 MECI geometry, which are useful for interpreting and predicting the MECI geometries of organic molecules.

We derived the approximate S_0-S_1 energy difference based on the frozen orbital analysis (FZOA) [1], which restricts the excited configurations to the minimum active space. In spin-conserved time-dependent density functional theory (TDDFT), the reference state is the closed-shell configuration determined by solving the Kohn−Sham equation, and (2e, 2o) active space is adopted. By comparing the components of the approximate excitation energy, numerical calculations unveiled the following relationships [2]:

$$\left|\Delta\varepsilon_{\mathrm{HL}} - J'_{\mathrm{HL}}\right| \approx 0, \quad K_{\mathrm{HL}} \approx 0,$$

where $\Delta\varepsilon_{\mathrm{HL}}$, J'_{HL}, and K_{HL} are the HOMO−LUMO gap, HOMO−LUMO Coulomb integral contribution, and HOMO−LUMO exchange integral, respectively.

Spin-flip TDDFT is a single-reference method that is capable of treating static correlation. The approximate S_0-S_1 energy difference for spin-flip TDDFT with restricted open-shell reference state was derived. The interpretable formula was obtained when using appropriate coupling coefficients for orbital energies. Numerical calculations identified the following relationships [3]:

$$\Delta\varepsilon_{\mathrm{HL}} + J''_{\mathrm{HL}} \leq 0, \quad K_{\mathrm{HL}} \approx 0,$$

where J''_{HL} is the contribution of Coulomb integrals. Note that the small HOMO−LUMO exchange integral can be used as a constraint in the geometry optimization of MECIs, as reported in literature [4].

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Research Interests

- Computational Chemistry
- Chemoinformatics
- Computational Science
- High-Performance Computing

Computational Modeling of Ground-State Electronic Structure and X-ray Spectra in Transition-Metal Sulfides

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Transition-metal sulfides show a wide range of chemical and electronic properties. These systems play a crucial role in advanced technologies and also serve as highly efficient catalysts in the active sites of biological enzymes. A remarkable example is the FeMo-cofactor in the nitrogenase enzyme of bacteria, which enables the conversion of nitrogen gas into ammonia under ambient conditions. This exceptional catalytic activity is believed to lie in its complex and strongly correlated electronic structure.

To explore the electronic property of the FeMo-cofactor, we have performed the ground-state electronic-structure simulation of the cluster, using the active space model. Employing the density-matrix renormalization group algorithm, along with the matrix-product-state (MPS) representation of the active-space wavefunction, has yielded insightful findings. Notably, we have observed extremely strong correlation in the ground state. [1] Intriguingly, our simulation suggests that the Mo atom in the cluster could function as an electron pump, pushing electrons to the Fe atoms, potentially enhancing nitrogen gas binding.

The validity of the theoretical active-space model can be assessed by comparisons of X-ray spectra from experiments and theoretical simulations based on the active-space model. We considered L-edge X-ray absorption spectroscopy (XAS) and 2p3d resonant inelastic X-ray scattering (RIXS) spectroscopy. These spectroscopies provide high-intensity and high-resolution spectra, capturing the complex phenomena of electron correlation, ligand-field splitting, and multiplet splitting, spin-orbit splitting, etc. We have developed a novel approach to simulate the spectra of transition-metal sulfides, which overcomes several challenges using the correction vector formulation and MPSs. [2] We achieved the first successful spectra simulation for iron-sulfur clusters. This breakthrough enables the correction of a previously misassigned experimental RIXS band, highlighting the significant role of ligand-to-metal charge transfer (LMCT) in the cluster. Moreover, the analysis of similarities and differences between experimental and theoretical spectra allows us to rigorously validate the strength and the limitation of the theoretical model. We believe these novel techniques will advance our understanding of the electronic structures of transition-metal sulfides.

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Research Interests

- Quantum Chemistry
- Ab-Initio Electronic Structure Method
- Strong Electronic Correlation
- Quantum Computing Algorithm

Interdisciplinary Applications of Computational Chemistry in Materials Science

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Computational and theoretical chemistry represent a fundamental pursuit to understand chemical phenomena through mathematical modeling and physical principles. In particular, quantum chemistry, provides insights at the molecular and electronic levels that enable us to interpret and predict physical and chemical phenomena in diverse systems. Among various methods, density functional theory (DFT) has become the most widely used due to its balance between computational efficiency and accuracy, thereby extending its influence beyond traditional quantum chemistry into broader areas of materials science. In this presentation, I will introduce several recent studies where computational chemistry has guided the development of advanced energy materials through theoretical understanding. These examples demonstrate how computational chemistry serves as a design engine that connects theory with synthesis and experiment. Despite the remarkable progress, the intrinsic accuracy limits of current DFT approaches call for paradigm shifts toward emerging methodologies, including artificial intelligence-assisted modeling and quantum computing-based simulations. Finally, I will briefly discuss perspectives on how the field of computational chemistry can evolve to meet these new challenges and opportunities across interdisciplinary research domains [RS-2024-00443714].

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Tensor-Product Bitstring Selected Configuration Interaction

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Selected configuration interaction (SCI) methods are effective for strongly correlated systems but have long been limited by software implementations that replicate the configuration interaction (CI) vector across processes.

Here, we overcome this limitation by developing the first SCI implementation with fully distributed CI vector storage, based on a tensor-product bitstring construction. We denote this method as tensor-product bitstring SCI (TBSCI).

Integrated with a novel bitstring-based algorithm and a suite of MPI communication strategies, TBSCI can efficiently handle 2.6 trillion determinants on Fugaku—exceeding the previous SCI record by three orders of magnitude. Moreover, for all tested molecules, TBSCI based on FCI-derived bitstrings yields energies close to the FCI results with only a tiny fraction of the Hilbert space. These results establish a scalable, physically motivated strategy for SCI, opening a new computational frontier in quantum chemistry.

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Development of Valence Bond Methods and Algorithms

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Valence bond (VB) theory is inherently a multi-configuration approach, well-suited for treating strongly correlated systems. A VB structure, constructed from nonorthogonal atomic orbitals, directly corresponds to a Lewis structure, providing unique physical insights that align with classical chemical concepts and revealing the intrinsic nature of chemical bonds. Additionally, VB theory is an effective framework for constructing diabatic states.

Despite its strengths, the widespread application of VB theory is hindered by its higher computational cost compared to molecular orbital (MO) theory. In this presentation, we focus on our recently developed VB methods and algorithms, which address this limitation:

1. Efficient algorithms for VB theory with nonorthogonal orbitals, including biorthogonal transformations, low-rank algorithms for electronic integrals, and analytical energy gradient evaluations.
2. The hybrid DFVB method and its multistate extension, which are multireference density functional theory (MRDFT) approaches that incorporate both static and dynamic correlation. The multistate extension allows for the calculation of both adiabatic and diabatic states.
3. A deep learning framework that integrates VB theory with graph transformers through a chemically interpretable representation of VB structures. The regression model predicts VB structure weights without requiring ab initio calculations, while the classifier model automatically selects the most relevant VB structures for ab initio VB computations.

Keywords：valence bond theory, algorithms for nonorthogonal orbitals, density functional valence bond method, deep learning valence bond method

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Research Interests

Methodology and algorithm development for strongly-correlated systems, including valence bond theory and multi-reference density functional theory.

Unraveling the Catalytic Mechanism and Substrate Selectivity of HDAC10: A Dual-Filter Approach for Polyamine Deacetylation

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The histone deacetylase (HDAC) family plays a crucial role in regulating acetylation-dependent cellular processes, with dysregulation linked to diseases ranging from cancer to neurodegeneration. HDAC10, the sole polyamine deacetylase in the HDAC family, uniquely influences pathologies such as tumor immunity, autophagy, inflammation, virus infection, silicosis, *etc*. Despite its therapeutic potential, the molecular basis of HDAC10's catalytic activity and substrate selectivity remains poorly understood, hindering rational drug design. Here, we address this gap by integrating density functional theory (DFT) and molecular dynamics simulation to systematically investigate HDAC10's catalytic activity and substrate selectivity. Utilizing a 330-atom quantum cluster model, we evaluated five distinct reaction pathways. The double-proton transfer mechanism (D'D) is dominant, featuring a concerted double-proton transfer step and a rate-limiting protonation of the substrate's amide nitrogen (20.4 kcal/mol barrier). Substrate selectivity arises from synergistic effects: N^8-acetylspermidine benefits from enhanced binding via active-site hydrogen-bond networks and reduced catalytic barriers compared to N^1-acetylspermidine, which suffers from electrostatic repulsion and dynamic instability. This study provides the first atomic-resolution framework for HDAC10's catalysis and selectivity, resolving long-standing mechanistic ambiguities. By identifying critical interactions governing substrate recognition and turnover, our work establishes a foundation for designing isoform-specific HDAC10 inhibitors, offering strategic avenues to target its roles in disease.

New Insights into Li^+/Mg^{2+} Separation by A CNT Model Membrane via Coupling High-Throughput Simulations and Machine Learning

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Membrane separation technology, due to its sustainability and cost-effectiveness, has been widely used for lithium extraction from salt lakes. In order to understand the separation mechanism of Mg/Li through nanofiltration membranes, high-throughput molecular dynamics simulations were performed in this work, by adjusting pore size, hydrophilicity, and membrane surface charge. The pore-size sieving effect is dominant for separating Li^+ and Mg^{2+}, from both molecular and machine learning analysis. Meanwhile, extremely high hydrophilicity of membranes will preferential allow Mg^{2+} to permeate due to the induced smaller hydration shell. More interestingly, the ion pair of Mg^{2+} and Cl^- will allow Mg^{2+}, rather than Li^+, to permeate through positively charged membranes. The machine learning results indicate that pore-size sieving has the greatest contribution to the Li/Mg selectivity. Moreover, if pore-size sieving effect is coupled with surface charge, this coupled factor will dominate the separation performance. The combination of high-throughput simulations and machine learning in this work provides a new approach for designing membrane materials to extract lithium from salt lakes.

Keywords: high-throughput molecular dynamics; machine learning; membrane surface charge; pore size; hydrophilicity

UAIQM – the Ultimate Solution to the Universal AI Models for Atomistic Simulations beyond DFT

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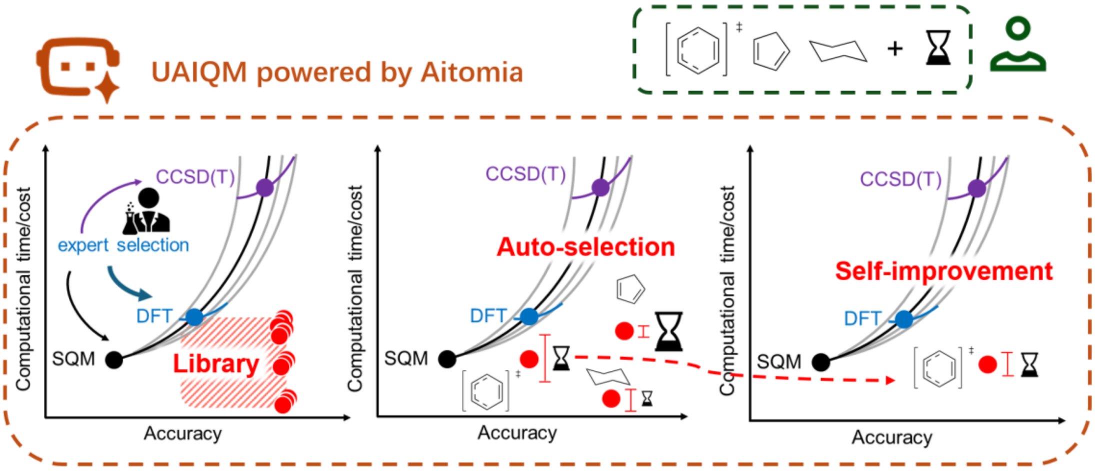
In this work, we introduced UAIQM [1], which is a platform hosting a library of foundational models ranging from universal machine learning interatomic potentials (UMLIPs) to AI-enhanced QM methods. The philosophy behind UAIQM is to automatically provide the best solution from the library according to the time budget and chemical system, and upgrade itself with those unreliable predictions. Up to now, models from the UAIQM library have shown accuracy and speed superior to or close to DFT in various tasks, including transition state optimizations, reactive molecular dynamics [2], and infrared spectra simulations [3]. Fine-tuning the established models for specific applications is also supported [4]. Simulations with AIQM models can also be performed autonomously by AI agents integrated in our in-house intelligent assistant, Aitomia [5].

A selection of the calculations with UAIQM (e.g., AIQM1 and AIQM2) can be performed using open-source MLatom (http://mlatom.com). The full support for the UAIQM library methods is provided via Aitomic add-ons (http://mlatom.com/aitomic/). The upgraded version supercharged by Aitomia is currently available online at https://www.aitomistic.xyz.



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Phonon-Mediated Ultrafast Energy- and Momentum- Resolved Hole Dynamics in Monolayer Black Phosphorus

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Electron-phonon scattering plays a crucial role in determining the electronic, transport, optical, and thermal properties of materials. In this work, we employ a non-Markovian stochastic Schrödinger equation (NMSSE) in momentum space, combined with ab initio calculation of energy bands and electron-phonon interactions, to investigate the ultrafast hole relaxation dynamics mediated by phonons in the valence bands of monolayer black phosphorus. Our simulations reveal that the hole can initially remain in the high-energy valence bands for over 100 fs, owing to weak interband scattering. Upon scattering into low-energy valence bands, the energy relaxation follows a single-exponential decay toward the valence band maximum. The total hole relaxation time is found to be significantly longer than that of electron in the conduction band, suggesting that harnessing the excess energy of holes may be more effective than that of electrons. Compared to the semiclassical Boltzmann equation based on a hopping model, the NMSSE captures prolonged quantum coherence, which substantially influences the relaxation dynamics. These findings complement the understanding of hot carrier relaxation dynamics in two-dimensional materials and may offer novel insights into harnessing hole energy in photocatalysis.

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Theoretical Simulations of Steady-State and Time-Resolved X-Ray Absorption Spectroscopy for Complex Systems

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X-ray absorption spectroscopy (XAS) serves as an element-specific probe of local electronic and geometric structure. Advances in X-ray light sources are enabling increasingly sophisticated experiments, generating a strong demand for accurate theoretical simulations to interpret spectral fingerprints. Modeling XAS for complex excited-state systems presents a particular challenge, as it necessitates both high-level electronic structure methods and the ability to describe nuclear dynamics. Here, we have developed an effective strategy by employing the multi-reference restricted active space configuration interaction (RASCI) method with large active space for steady-state XAS calculations. To capture ultrafast dynamics, we combined surface hopping simulations with XAS calculations for real-time XAS maps, tracing the non-radiative decay of pyrazine from its optically excited state B_{2u} ($\pi\pi^*$). Currently, our approach establishes its robustness through benchmarking on pyrazine, providing a foundation for accurate predictions of steady-state XAS for pentacene. For the time-resolved application, the completed surface hopping simulations have revealed the key non-radiative decay dynamics. We are now integrating these trajectories with XAS calculations to generate the time-resolved spectral maps, which will provide a direct link between the structural dynamics and experimental observables.

Exciton Dynamics in Edge-on ZnPc–F_8ZnPc System: Insights from Quantum Simulations

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Focusing on the mechanism of interfacial exciton dissociation in edge-on stacked ZnPcF_8–ZnPc aggregate, we employed the fragment particle-Hole densities (FPHD) method to construct the Hamiltonian of diabatic states and used the Non-Markovian Stochastic Schrödinger Equation to simulate the photo-induced dynamic processes. The results show that aggregation effects have a significant impact on the interfacial exciton dissociation process. After photo-excitation, the excitions first preferentially delocalize and perform the charge transfer states in the pure ZnPc or F_8ZnPc aggregates within 100 fs. These 'intramolecular' charge transfer (CT) states can easily evolve into interfacial CT states by hopping of electrons and holes in the intramolecular CT states across the interface. Comparing with these processes, the direct exciton dissociation into interfacial CT state is relatively slow due to the small electronic coupling and vibrational coherence between the locally excited state and the interfacial CT state. As the temperature rises and the vibronic coherence weakens, the direct dissociation rates are significantly enhanced. This investigation provides valuable insights for the design and optimization of high-performance organic photovoltaic devices.

Keywords: ZnPc-F_8ZnPc, Exciton dynamics, Delocalization and coherence effects, vibronic coupling effects

Multireference Block-Correlated Coupled Cluster Theory with up to Five-pair Correlation

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To describe electronic structures of strongly correlated systems with singlet ground states, we have proposed generalized valence bond based block-correlated coupled cluster theory with up to five-pair correlation (GVB-BCCC5). Several efficient techniques are employed to make GVB-BCCC5 calculations practical for strongly correlated systems. We then apply this method to investigate various systems, including potential energy surfaces of a hydrogen cuboid lattice and a phosphorus cluster (P_4), relative energies of two isomers for C_8 and V_2H_2, the bond dissociation energy in a metal-oxide compound, FeO_3. All calculations show that GVB-BCCC5 can provide nearly exact static correlation energy as the density matrix renormalization group (DMRG) method (based on the same GVB orbitals). This work demonstrates the potential applications of the GVB-BCCC5 method in the accurate description of many strongly correlated systems.

Development of Gaussian Charge Distributed Harmonic Solvation Model

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Chemical reactions proceed in various environments such as gas phase, liquid phase, solid phase, and on solid surfaces. Thermodynamic quantities governing the directions and equilibrium states of chemical reactions, as well as activation barriers determining the reaction rates are defined by changes in Gibbs or Helmholtz free energies. Although the electronic energy of a system obtained from quantum chemical calculations based on the Born-Oppenheimer approximation account for the majority of the free energy, the evaluation of entropy is essential for understanding the temperature dependence of chemical reactions. Computations of Gibbs energies in gas phase with the help of statistical mechanics have been implemented in most quantum chemical program packages. One of the authors (HN) previously pointed out that this scheme cannot accurately estimate the free energy in solution due to the overestimation of entropy, and proposed an alternative model that incorporates the interactions with the solvent in a harmonic manner, referred to as harmonic solvation model (HSM) [1]. However, since the previously proposed HSM, which adopts the standard polarizable continuum model (PCM) using point charges on the tessellated cavity surface, as denoted by PC-HSM, occasionally leads to unphysical imaginary frequencies. In this study, we modify the HSM by replacing point charges with Gaussian charges as used in a Gaussian charge model (GCM) [3], thus, refer to the modified model as GC-HSM. Illustrative applications confirmed that the new model successfully eliminates imaginary frequencies. In the presentation, we will demonstrate the formulation of GC-HSM and its illustrative applications.

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Aitomia: AI Agents for Autonomous AI-Driven Atomistic Simulations

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We have developed Aitomia – a platform powered by AI to assist in performing AI-driven atomistic and quantum chemical (QC) simulations. It performs AI-driven simulations covering both ground and excited states, including geometry optimization, thermochemical analysis, and spectral computations, making such simulations more adaptive and practically feasible. The multi-agent implementation enables autonomous executions of the complex computational workflows, such as the computation of reaction enthalpies, and automated spectral calculation. By integrating large language models with the MLatom ecosystem, Aitomia is expected to lower the barrier to performing AI-Driven Atomistic and Quantum Chemical Simulations, thereby accelerating research and development in relevant fields.

Construction of fused BN-heterocycles *via* boron atom insertion: DFT insights into the Lewis acid–base (BBr_3/NEt_3) cooperative mechanism and selectivity

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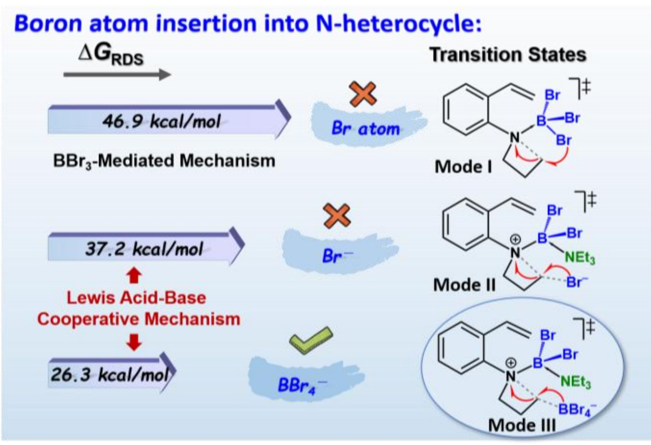
The BBr_3-mediated N-heterocycle editing reaction through a boron atom insertion strategy reported by Song et al. (*Angew. Chem., Int. Ed.*, **2024**, 63, e202318613) has been systematically explored using density functional theory (DFT) calculations. The present results reveal that in addition to BBr_3 acting as a boron source and an electrophile, the Lewis base NEt_3 also plays a crucial role. Specifically, the Lewis acid–base cooperative interaction between BBr_3 and NEt_3 facilitates the ring-opening of the substrate 1-(2-vinylphenyl) azetidine, the rate-determining step of the overall cascade reaction. Notably, the organic base NEt_3 facilitates the formation of the real nucleophilic species BBr_4^-, thereby promoting the progression of the reaction. Furthermore, the formation of an exceptionally stable C_4NB π-ring intermediate and the difference in distortion and exchange-repulsion energies, caused by structural characteristics of substrates, are responsible for the chemoselectivity and regioselectivity of substrates bearing typical structural motifs and functional groups, respectively. These computational findings not only provide profound mechanistic insights into the tandem reactions involved in the construction of fused BN–heterocycles, but also elucidate the underlying factors governing substrate preference.



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Time-Dependent Kohn−Sham Electron Dynamics Coupled with Nonequilibrium Plasmonic Response via Atomistic Electromagnetic Model

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Computational modeling of plasmon-mediated molecular photophysical and photochemical behaviors can help us better understand and tune the bound molecular properties and reactivity, as well as make better decisions in designing and controlling nanostructures. However, computational investigations of coupled plasmon–molecule systems are challenging due to the lack of accurate and efficient protocols for simulating these systems. Here, we present a hybrid scheme that combines the real-time time-dependent density functional theory (RT-TDDFT) approach with the time-domain frequency-dependent fluctuating charge (TD-ωFQ) model. The ωFQ model, an atomistic electromagnetic model for the plasmonic response of plasmonic metal nanoparticles (PMNPs), is first transformed into the time domain and described by an equation-of-motion formulation. Then, TD-ωFQ is combined with RT-TDDFT, in which TD-ωFQ introduces the nonequilibrium plasmonic response of PMNPs and atomistic interactions to the electronic excitation of the quantum mechanical (QM) region. As a first application of the RT-TDDFT/TD-ωFQ method, we study the nonradiative decay rate and plasmon-enhanced absorption spectra of two small molecules in proximity to sodium MNPs. Thanks to the atomistic nature of the ωFQ model, the edge effect of MNPs on absorption enhancement has also been investigated and revealed. In another example, consisting of a sodium spherical-nanoshell dimer and a quantum emitter, we tune the coupling strength by changing the molecular orientation relative to the dimer axis. It is shown that the induced dipoles evolve from an exponential decay pattern to a beat pattern as the coupling strength increases. It is further shown that in the strong coupling regime, both the excited molecule and the plasmon relax rapidly due to the molecule–plasmon interaction, and efficient coherent energy exchange between the interacting molecule and plasmon modes occurs on a femtosecond (fs) timescale. The TDDFT/TD-ωFQ method allows us to effectively simulate

plasmon-mediated real-time electronic dynamics and even coupled electron–nuclear dynamics by combining it with nuclear dynamics approaches. This study significantly contributes to understanding the dynamic responses of nanoscale systems and provides guidance for further enhancing coupling strength, as well as exploring new materials and structures for strong coupling and for practical applications in optoelectronics and quantum technologies.

Theoretical Study on Dynamically Hidden Reaction Path: Dissociation of C+ from Doubly Ionized OCS

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I. Introduction

The global reaction route mapping (GRRM) strategy enables the construction of reaction path networks consisting of intrinsic reaction coordinates (IRCs) based solely on potential energy surfaces (PESs) [1]. However, these analyses neglect molecular dynamics effects. By performing ab initio molecular dynamics (AIMD) simulations, Hase and co-workers discovered a non-IRC process, and Tsutsumi et al. identified a phenomenon in which trajectories moving near one IRC transfer to another nearby IRC, which they termed an IRC-jump process [2]. While such processes involve molecular motion through regions where no IRC exists, the reverse case – where the system fails to follow an existing IRC – has also been reported. Oda et al. found that when a subsequent reaction proceeds before the intermediate reaches equilibrium, the pathway to the intended product becomes inaccessible. They termed this a dynamically hidden reaction path [3]. In this study, we focus on the hidden process in the fragmentation of photo-induced OCS^{2+}, extending the analysis to the excited-state processes. For this species, dissociative channels yielding CO^{+} + S^{+} and CS^{+} + O^{+} have been observed, and the involvement of the COS^{2+} isomer has been proposed experimentally; however, OS^{+} + C^{+} has not been observed [4].

II. Method

All analyses were performed by comparing static PESs with dynamical effects. For the ground state, GRRM searches and AIMD simulations were conducted. For the excited states, potential energy curves (PECs) were constructed, and nonadiabatic surface-hopping (SH-) AIMD simulations were carried out using our in-house program SPPR [5].

III. Results and Discussion

In the ground-state reaction path network, the COS^{2+} isomer was identified as a local minimum. However, in AIMD simulations, no trajectories reached this geometry, hindered by the inertia associated with CO+ rotation. For the excited states, after constructing the PECs, several electronic states were selected as initial states based on their molecular orbitals and dominant electronic configurations. In the presentation, we will discuss the vibronic coupling and dissociation dynamics in detail [6].

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Revealing Common Nature of O And S Doping in Enhancing the Oxygen Electrocatalytic Performance of FeN4

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The development of oxygen reduction reaction (ORR) catalysts is an important and challenging topic in the fields of energy and materials. Fe-N-C catalysts are promising alternatives to platinum-group metals due to their low cost and high activity. However, there is a trade-off between the activity and stability of Fe-N-C catalysts. O and S dopings can effectively enhance their ORR catalytic performance, but the underlying reasons are not clear yet. By constant potential implicit solvent model, we revealed that in acidic environments, pyrrolic FeN4 is prone to protonation, leading to the dissolution of Fe and rapid deactivation. Conversely, in alkaline environments, the axial coordination of Fe enhances the stability and activity of pyridinic FeN4. This finding explains experimental observations under acidic and alkaline conditions. Furthermore, we found that under acidic conditions, O and S heteroatoms effectively reduce the protonation ability of pyrrolic N, and improve the ORR catalytic activity of pyridinic FeN4. Under alkaline conditions, the catalytic activity of both pyridinic and pyrrolic structures was effectively enhanced. Through in-depth mechanistic analysis, we found that the multi-electron properties of O or S enhance their conjugation with coordinating N and Fe, significantly reducing the intrinsic protonation ability of pyrrolic N by reducing its pDOS at the Fermi level. Additionally, the downward shift of the p orbital energy level of intrinsic pyridinic N reduces the d-band center of Fe, thereby adjusting the adsorption behavior of intermediates and significantly increasing the catalytic activity of pyridinic FeN4C while ensuring stability. Moreover, doping with O and S strengthens the catalytic activity of FeN4C catalysts in alkaline environments through such conjugation effects. This study identifies the common characteristics of O, S, and other multi-electron atoms in enhancing the oxygen electrocatalytic function of FeN4, providing theoretical guidance for the rational design of Fe-N-C catalysts with enhanced durability and activity.

Variational Quantum Simulation of Time-Local Quantum Master Equations via Quantum Jump

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Strong coupling and environmental memory render many open quantum systems intractable to classical computation. To overcome this barrier, we present a variational quantum algorithm capable of solving generalized form time-local quantum master equations directly on Noisy Intermediate-Scale Quantum (NISQ) processors. The resulting protocol remains resilient under realistic hardware noise. We validate it on both classical simulators and a 66-qubit superconducting processor for solving Redfield master equation and fourth-order time-local non-Markovian master equation and find that it can successfully capture key features of complex open quantum dynamics-including non-Markovian oscillations and strong coupling effects. Our approach establishes a practical pathway toward scalable simulations of open quantum systems in the NISQ era.

MXenes Enhance Electrocatalytic Water Electrolysis of NiFe Layered Double Hydroxides Through Bifunctional Heterostructuring

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Transition metal-based layered double hydroxides (TM-LDHs) are among the most promising catalytic materials for the electrochemical reactions involved in energy conversion and storage technology. We systematically investigate NiFe-LDH-based electrocatalysts toward application in water electrolysis. We start with the highly accurate advanced density functional theory description of NiFe-LDH's fundamental properties, and demonstrate that coupling a spin-polarized p-band or d-band center model with the Gibbs free energy calculations explains NiFe-LDH's oxygen evolution reaction (OER) mechanism. By involving the related transient states, a reversible oxygen vacancy assisted reaction mechanism has been directly observed and motivated by the high spin transition metal impurity which is further confirmed by the time-consuming hybrid functional method. To further facilitate the electrocatalytic activity of NiFe-LDH, we study NiFe-LDH/MXene heterostructures where the essential semiconductor-to-metallic transition takes place by the additional Ti-3d orbitals and the interfacial non-covalent interaction between the two catalysts. On the basis of calculated results, we propose a link between microscopic properties and macroscopic electrocatalytic kinetics of heterogenous electrocatalysts. Accurately describing the electronic and magnetic structures of electrocatalysts leads us to a step-by-step process for tailoring desired electrocatalytic properties, especially for the high spin state contained TM-LDHs. A descriptor based on combination of the calculated d-band center of transition metal and p-band center of oxygen is the key to predicting electrochemical activity and stability of oxide electrocatalysts. From our results, we establish a design strategy for NiFe-LDH-based bifunctional electrocatalyst fabrication. [1]

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Multi-Scale Mechanisms Reveal the Synergistic Strategy of Remote Mutations in MPH Enzyme for Enhancing Stability and Activity

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In traditional enzyme engineering, balancing catalytic activity with thermostability remains a significant challenge. Engineered methyl parathion hydrolase (MPH) variants such as MPHase-m5a and MPHase-m5b exhibit simultaneous improvements in both properties, while the underlying cooperative mechanisms remain elusive. To address this, pocket dynamics, molecular dynamics simulations, and QM/MM calculations were applied to investigate how distal mutations reshape structural dynamics and catalytic pathways of MPH. By reconfiguring the active-site microenvironment, these mutations redirect substrate binding to the right pocket and convert a strictly water-mediated hydrolysis into a dual pathway, with catalysis proceeding either by direct attack from a bound water or by a bridging hydroxide. Furthermore, long-range allosteric interactions enable temperature-sensitive regulation of enzyme thermostability. Two distinct allosteric engineering strategies were identified: MPHase-m5a enhances thermostability through local rigidification, whereas MPHase-m5b employs dynamic decoupling to preserve cooperative networks while facilitating efficient product release, thereby boosting catalytic efficiency. This work establishes a structure-dynamics-function relationship for distal mutations in MPH and provides a rational design strategy applicable to MPH and other structurally homologous hydrolases.

Keywords: Pocket dynamics, QM/MM, Enzyme thermostability, Enzyme mutagenesis

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Rational Design of Transition Metal–Phosphorus Dual-Atom Catalysts in Defective h-BN for CO_2 Hydrogenation and Cycloaddition

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In this study, density functional theory (DFT) calculations and ab initio molecular dynamics (AIMD) simulations were employed to design transition metal–phosphorus dual-atom catalysts (M_1–P_1/V_{BN}, M = Ir, Rh, Co) supported on defective hexagonal boron nitride (h-BN). The catalytic mechanisms of CO_2 hydrogenation and cycloaddition reactions were systematically investigated. The results reveal that the metal–phosphorus dual sites cooperatively activate CO_2 and H_2 during hydrogenation, and CO_2 and propylene oxide (PO) during cycloaddition, thereby facilitating the formation of formic acid (HCOOH) and propylene carbonate (PC), respectively. By combining static calculations with microkinetic simulations, we show that Ir_1–P_1/V_{BN} and Co_1–P_1/V_{BN} exhibit superior catalytic activity for CO_2 hydrogenation, whereas Rh_1–P_1/V_{BN} displays the highest efficiency in cycloaddition. Screening of 3d transition metals further indicates that the adsorption strengths of small molecules strongly depend on the metal identity, and that linear scaling relationships exist among the adsorption energies of key intermediates. This work provides fundamental insights into the thermocatalytic CO_2 hydrogenation and cycloaddition mechanisms mediated by M_1–P_1/V_{BN} dual-atom catalysts, and highlights the great potential of h-BN–based materials for CO_2 conversion.

Keywords: CO_2 hydrogenation and cycloaddition, dual-atom catalysts, defective h-BN, multifunctionality, first-principles calculations

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PyMEDA: A Unified Python Framework for Multiscale Energy Decomposition Analysis

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Abstract: Energy decomposition analysis (EDA) has become a powerful approach for elucidating chemical bonding and non-covalent interactions, especially in complex and multiscale systems. Embedding strategies combining high-level quantum chemical methods with more approximate treatments of the environment provide a promising balance between accuracy and efficiency, yet existing embedding schemes of EDA approaches implementations are often fragmented and software-dependent. To address this challenge, we present PyMEDA, a unified, open-source interface framework for multi-scale energy decomposition analysis. Through a modular design, PyMEDA standardizes interfaces to diverse quantum mechanical, molecular mechanics, and semi-empirical backends (initially XEDA, OpenMM, and xtb), enabling the unified implementation of workflows for both conventional and embedding-type EDA schemes, such as DM-EDA(QM/MM) and DM-EDA(EB). By providing extensibility, reproducibility, and automation, PyMEDA offers a flexible environment to advance multiscale interaction analysis and facilitates the future development of embedding-based EDA methods.

A Theoretical Study on the Mechanism of Strain-Regulated Oxygen Evolution Reaction Performance of RuO_2

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Strain engineering effectively tunes the geometric and electronic structures of RuO2, enabling enhanced activity and stability toward the acidic oxygen evolution reaction (OER). However, the modulation mechanism induced by strain has not yet been fully elucidated. In this work, density functional theory calculation and machine learning methods are employed to systematically explore the effects of biaxial strain on the structural, electronic, and catalytic properties of RuO2. The results indicate that applying 5% tensile strain along the a-axis and 2% compressive strain along the b-axis attains optimal catalytic performance, with an overpotential of 0.623 V, representing a 22% improvement over the unstrained system. Based on a broader set of input features, XGBoost Regression (XGBR), Random Forest, Neural Network, Support Vector Regression models are constructed, among which the XGBR model achieves the best balance between predictive accuracy and interpretability. The Shapley Additive exPlanation analysis reveals that biaxial strain optimizes the reaction energetics of active sites by modulating key electronic structural parameters, thereby elucidating the microscopic origin of strain-enhanced OER activity.

Divide-and-Conquer MP2 for Periodic Systems

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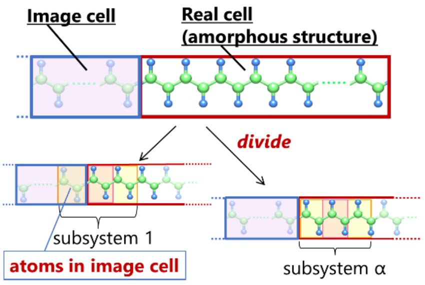
Hyper-ordered structures refer to unique nanoscale structures composed of dopants, vacancies, and voids. Elucidating the mechanisms underlying the functionality of such structures at the atomic level will open the development of next generation materials, and electronic structures calculations are expected to play an important role in elucidating these mechanisms.

It remains challenging to elucidate the functional manifestations of hyper-ordered structures through electronic structure calculations. When employing *ab initio* quantum chemical methods, which can systematically improve accuracy and are typically applied to isolated systems, it is necessary to construct large-scale cluster models to mitigate "edge effect." Similarly, when using condensed matter physics that treat periodic systems with DFT, constructing large-scale periodic models capable of adequately describing the amorphous structure is essential. Since there are few DFT methods that offer the same level of systematic improvements in accuracy as ab initio methods, there has been strong demand for developing large-scale periodic boundary condition (PBC) calculation method based on *ab initio* approaches.

We have developed divide-and-conquer (DC) Hartree-Fock (HF) and post-HF methods as accurate fragmentation-based calculation methods for large-scale isolated systems [1,2]. In this study, we extended the DC-HF/MP2 methods to periodic systems and developed the DC-HF/MP2-PBC program. This program leverages the features of the DC method to solve periodic systems using a real-space Gaussian basis (Fig.1), a strategy reminiscent of fragment molecular orbital (FMO) calculations with PBC [3].



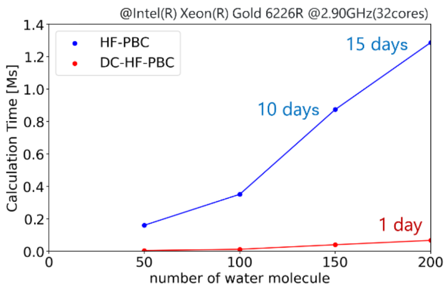


Figure. Subsystem construction for PBC and calculation time.

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Unitary Matrix Optimization in Quantum Chemistry with Givens Rotation and Error Backpropagation

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The self-consistent field (SCF) procedure is a standard method for solving Hartree–Fock and Kohn–Sham density functional theory calculations, although its convergence is not guaranteed. Direct minimization methods, such as the second-order SCF (SOSCF) [1], optimize molecular orbitals (MOs) using the gradient of the Lagrangian. In standard SOSCF calculations, MOs are updated via a truncated Taylor expansion of a unitary matrix expressed in exponential form, ensuring the orthonormality condition. Since the exponential is typically approximated by a first-order truncation, Gram–Schmidt orthogonalization is needed to restore unitarity.

We have recently developed a novel direct minimization method, referred to as the direct Givens rotation (DGR) [2], to obtain SCF solutions by combining the Givens rotation method with the error backpropagation (EBP) technique [3]. The Givens rotation, defined by a rotation angle, performs unitary transformations that inherently preserve orthogonality, thereby eliminating the need for Gram–Schmidt orthogonalization required in SOSCF. EBP is a differentiation technique based on the chain rule, frequently employed in neural networks, that algorithmically computes gradients from the output layer. The proposed DGR method evaluates complex gradients of the Lagrangian with respect to the rotation angle using the EBP technique. Illustrative applications demonstrate that the DGR method exhibits stable optimization behavior compared to conventional SCF algorithms, including direct inversion in the iterative subspace (DIIS) [4] and SOSCF. Its generality allows application to a wide range of orbital optimization problems based on unitary transformations, i.e., antisymmetric product of geminals wavefunction [5].

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Theoretical Insights into Exchange Coupling Interactions in Two Biomimetic Mixed-Valence Manganese Complexes: A DMRG Study

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Manganese complexes exhibiting magnetic interactions play a pivotal role in single-molecule magnetism and photosynthetic water oxidation. These systems often possess dense spin manifolds with energy gaps smaller than the threshold of chemical accuracy (1 kcal/mol), making the accurate theoretical description of their electronic structures and magnetic properties a significant challenge due to strong electron correlation effects. The state-of-the-art multi-configurational calculations with an extensive active space encompassing 31 electrons in 26 orbitals were used to investigate the electronic structures of two mixed-valence manganese dimers: $[Mn_2(\mu\text{-}O)_2(\mu\text{-}OAc)(tacn)_2]^{2+}$ and $[Mn_2(\mu\text{-}O)_2(\mu\text{-}OAc)(bpea)_2]^{2+}$ with the density matrix renormalization group (DMRG) method. The results demonstrate that DMRG provides superior accuracy over the widely used broken-symmetry density functional theory (BS-DFT) in predicting magnetic exchange coupling constants (J_{ij}). Our results establish DMRG as a critical tool for accurately predicting degenerate spin-state energetics and offer fundamental insights into the manipulation of exchange interactions in magnetically coupled metal systems, in which the magnetic coupling is mediated by ligand charge along the superexchange pathways.

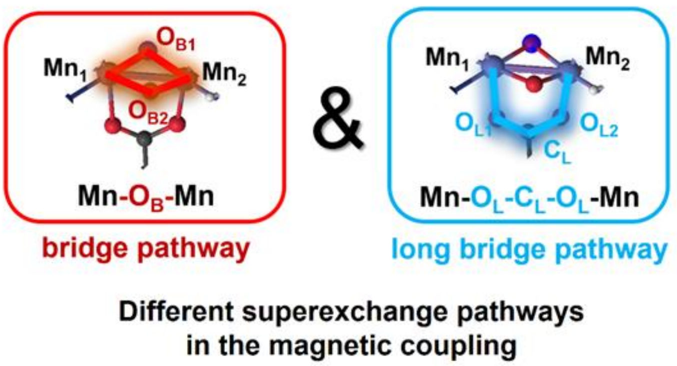

Figure 1. Schematic diagrams of the pathways in the Mn dimers.

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Efficient Evaluation of Spin-orbit Couplings in Single-molecule Magnets Using DMRG within The DMET Framework

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The accurate characterization of complex electronic structures in single-molecule magnets (SMMs) is crucial for guiding their rational design. However, conventional multireference wavefunction theory faces significant computational bottlenecks for these systems, stemming from their intricate ligand environments and the necessity for large active spaces to capture strong electron correlation. To overcome these limitations, we introduce an efficient quantum embedding framework that synergistically combines density matrix embedding theory (DMET) with ab initio density matrix renormalization group (DMRG). Relativistic spin-orbit coupling (SOC) effect is incorporated through a state-interaction procedure using the eXact two-component atomic mean-field spin-orbit (X2CAMF-SO) operator. Benchmarking on representative single-ion magnets confirms that our DMET-embedded DMRG-SI approach delivers results highly consistent with all-electron calculations, while offering a clear path for systematic improvement via active space expansion. Furthermore, by investigating SOC effects in a chromium dimer, we demonstrate the method's potential for high-accuracy and scalable ab initio studies of larger-sized polynuclear SMMs.

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Insights into Proton Transfer Dynamics in Histidine Tautomers of Amyloid-β (1-40)

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Histidine tautomerization within amyloid beta (Aβ) peptides is crucial in understanding the molecular mechanisms underlying Alzheimer's disease and its potential therapeutic strategies. Despite its significance, the proton transfer dynamics between histidine residues in Aβ-40 at the protein level remain insufficiently explored due to the complexity of solvent effects and the computational challenges of large-scale simulations. This study conducted fully quantum mechanical molecular dynamics (QM-MD) simulations coupled with metadynamics (MTD) to investigate the tautomerization process between histidine tautomers in Aβ-40 within an aqueous environment. Using the divide-and-conquer density-functional tight-binding (DC-DFTB) method, a system of ~3000 atoms was modeled to capture the atomic-scale interactions. MTD simulations revealed that water molecules mediate the tautomerization of histidine residues, HIS13 and HIS14, stabilizing specific tautomeric forms. The two-dimensional well-tempered MTD (2D WTMTD) results identified a reaction barrier of approximately 3.51 kcal mol-1 for tautomerization. This study represents the first comprehensive QM-MD/MTD investigation of histidine tautomerization in amyloid beta peptides, offering an insights into the tautomerization process.[1]

Reference

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Theoretical Study of Linearly fused Imide-functionalized Thienoacenes and Universal Machine Learning Potentials for Excited States

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Quantum mechanical (QM) excited-state simulations provide crucial insights into the process of electronic excitation and are powerful tools in the rational design of photochemical materials. In this work, the linearly fused **I**mide-functionalized **T**hieno**a**cenes (ITA) compounds with alternating donor-acceptor units were studied. Ground-state geometries were optimized using an AI-enhanced QM method - UAIQM$_{gfn2xtbstar@cc}$ in MLatom package, showing a good alignment with the crystal structure. TD-DFT calculations were performed based on the optimized geometries. The results show that thiophene units act as donors and NDI as acceptors during excitation. Simulated UV-vis spectra reveal only slight red shifts with conjugated unit expansion. Electronic-hole analysis indicates charge transfer from thiophene to NDI (major) alongside minor local excitations. This theoretical investigation could potentially contribute to the rational design of novel photochemical and electrochemical materials.

High-accuracy QM methods play a role in the discovery of novel photo-materials. However, the high computational costs of these methods make it difficult for large systems and large-scale screening. Universal machine learning potentials (UMLPs) provide near reference-level accuracy simulations at force-field cost. however, the development of excited-state UMLPs lags due to the electronic complexity of excited states. To develop UMLP for excited-state simulation, several excited-state databases were evaluated using the Multi-State ANI (MS-ANI) neural network. PubChemQC showed the best quality, enabling OMNI-P2x — the first UMLP for excited states that integrates MS-ANI and All-In-One frameworks. Now OMNI-P2x is available on Aitomistic Hub (https://aitomistic.xyz).

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A Template-Based Automatic Fragmentation Algorithm for Generalized Energy-Based Fragmentation Approach

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A major bottleneck in low-scaling energy-based fragmentation methods is the need for manual intervention in the fragmentation step, which is time-consuming, inconsistent, and hard to generalize across diverse molecular system. To address this challenge, we develop a template-based automatic fragmentation algorithm that extends the generalized energy-based fragmentation (GEBF) approach to a wide range of large and complex molecules. A hierarchical SMILES-encoded GEBF template library for both cyclic and acyclic functional groups enables chemically meaningful and efficient partitioning via structure conversion, macrocycle detection, substructure matching, and small-fragment merging. Controlling fragment sizes ensures a balance between accuracy and computational cost, while user-defined templates offer enhanced flexibility. Benchmarks on biomacromolecules, macrocycles, porous organic cages, polyamide oligomers, and ionic liquids reproduce conventional quantum-chemistry results within a few kcal/mol (or sub-meV/atom), while reducing the largest subsystem basis size to less than one-third of the full system. Experimental-level agreement is achieved in structural and spectroscopic predictions, and systems with ≈1,500 atoms are computed within practical timeframes. This work paves the way for fully automated, scalable, low-cost, high-accuracy quantum chemistry, bridging theory and large-scale real-world applications.

Development of High-Accuracy Diabatization Methods Based on Valence Bond Theory

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A common way to describe electronic structures near conical intersections (CIs) is through diabatic representations. Unlike conventional molecular orbital methods, valence bond (VB) theory uses localized atomic orbitals to construct VB structures corresponding directly to Lewis bonding patterns, providing a natural framework for constructing diabatic states with clear chemical interpretability. Most existing diabatization methods are based on MCSCF wavefunctions without dynamic correlation. Since systems near CIs are strongly correlated, an accurate description requires a balanced treatment of both static and dynamic correlations. To address this, we developed two VB-based diabatization methods that explicitly incorporate dynamic correlation:λ-DFVB(MS) and L-VBPT2.

In the λ-DFVB(MS) approach, VB diabatic states are first generated using the valence-bond-based compression approach for diabatization (VBCAD). Dynamic correlation effects are then introduced through density functional theory (DFT), yielding an effective Hamiltonian matrix constructed on the VB diabatic basis. The interactions among diabatic states are subsequently recovered by diagonalizing this effective Hamiltonian. Benchmark calculations demonstrate that the λ-DFVB(MS) method accurately reproduces the potential energy surfaces of both adiabatic and diabatic states in CI regions and outperforms XMS-CASPT2 in describing the avoided crossing of LiF.

The L-VBPT2 method, derived from the XMS-VBPT2 framework, employs the dynamically correlated wavefunction from localized-orbital XMS-VBPT2 as the starting point for VBCAD. Consequently, L-VBPT2 provides highly accurate diabatic energies, diabatic wavefunctions, and inter-state couplings, all incorporating dynamic correlation effects, while λ-DFVB(MS) yields only the diabatic energies. Currently, the implementation of the XMS-VBPT2 framework has been completed. In future work, the first-order corrected wavefunction from XMS-VBPT2 will be employed in the VBCAD procedure to generate dynamically correlated diabatic states.

Keywords：Valence Bond Theory；Diabatic State；Multistate；Hybrid Density Functional Valence Bond Theory； Valence Bond Second-Order Perturbation Theory

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Theoretical Study on Graphdiyne-Supported Cyclo[16/18] Carbon for Application in Lithium-Ion Batteries

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Developing safe and efficient energy storage systems is essential for the large-scale utilization of renewable energy. Lithium-ion batteries (LIBs) possess high energy density and long cycle life, making them widely used in portable electronics and electric vehicles. However, their cycling stability and rate capability remain insufficient for next-generation energy storage applications. In this study, a zero-dimensional/two-dimensional (0D/2D) heterostructure composed of cyclo[16/18] carbon and graphdiyne ($C_{16/18}$-GDY) is constructed as a novel high-performance anode material for LIBs. Both GDY and $C_{16/18}$ contain unsaturated diacetylene bonds, leading to electron accumulation in the stacking regions and providing abundant adsorption sites for lithium ions. Theoretical calculations reveal that lithium ions preferentially adsorb within the interlayer region, exhibiting ultralow diffusion barriers and high theoretical capacity. Band structure analysis shows that C16 contributes more electronic states near the valence band maximum (VBM), indicating higher charge transfer activity and thus stronger lithium adsorption capability. This work elucidates the interfacial electronic characteristics and lithium-storage mechanism of the $C_{16/18}$-GDY heterostructure, offering theoretical insights and rational design guidance for the development of high energy density and stable lithium-ion battery anodes.

Electronic Absorption and Circular Dichroism Spectra of One-Dimensional Bay-Substituted Chiral PDIs: Effects of Intermolecular Interactions, Vibronic Coupling, and Aggregate Size

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Electronic circular dichroism (ECD) spectroscopy is the preferred tool for studying organic chiral supramolecules. However, it is a great challenge to experimentally clarify the contributions to ECD spectra from molecular vibrational motions and the intermolecular interactions, key factors for an efficient system architecture design of chemical sensors, catalysts, or optoelectronics. Focusing on this issue, here, we perform theoretical studies on the vibrationally resolved absorption and ECD spectra of two one-dimensional bay-substituted chiral perylene diimides (PDIs) by employing the non-Markovian stochastic Schrödinger equation (NMSSE) with respect to the model Hamiltonian in the diabatic representation, which includes the intramolecular localized excited states (LEs), intermolecular change-transfer excited states (CTEs), and the vibronic couplings (VC) as well. Our calculated results exhibit that the theoretical spectra, with the inclusion of the VC effect, agree better with the experimental ones than those without this effect and that the difference between the traditional absorption spectra of the two bay-substituted PDIs is much less obvious than that in their ECD spectra, verifying that ECD spectroscopy is sensitive to the absolute configuration and conformation of chiral supramolecules. We further make a comparison among the pure electronic spectra of aggregates with different aggregate sizes calculated by the time-dependent density functional theory and the mixed exciton model with and without decoupling the LE and CTE states. It is shown that the hybridization between LE and CTE states results in the emergence of new peaks or troughs in the high-energy band and a significant deviation between the calculated ECD spectrum and that predicted by the exciton chirality rule. It is further shown that the ECD spectra of oligomers exhibit an odd–even alternation pattern with changes in aggregate size.

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Rationally Computational Engineering Diisopropyl Fluorophosphatase for Novichok A234 Detoxification

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Novichok nerve agents (A-type agents) exhibit significantly higher toxicity compared to traditional organophosphorus nerve agents, creating a daunting challenge for degradation research. Conventional approaches, whether reliant on metal-organic frameworks (MOFs) or small molecules, are often hampered by inadequate efficiency and poor environmental profiles. Against this backdrop, biodegradation stands out as a compelling alternative pathway.

In this study, combined with molecular dynamics (MD), quantum mechanics/molecular mechanics (QM/MM) calculations, and umbrella sampling to reveal that the hydrolysis of A234 by wild-type diisopropyl fluorophosphatase (DFPase) is inefficient—a limitation attributed to restricted active-site architecture and a suboptimal internal electric field. Rationally tuning the electric field (strength and direction) and enlarging the active pocket via introducing four-point mutations into DFPase, we achieved a catalytically enhanced variant. These findings are supported by multi-scale analyses that highlight several key mechanistic features: 1) Substrate transport and binding are more efficient in the variant than in the wild-type; 2) The optimized internal electric field lowers the hydrolytic barrier; 3) The enlarged active pocket admits a nucleophilic water, facilitating A234 hydrolysis with a modest barrier (12.8 kcal/mol) and strong exothermic drive (8.9 kcal/mol); 4) The stability of the variant and its reconfigured active pocket is confirmed through detailed pocket dynamics simulations.

Our theoretical simulations collectively show that a synergistic electric field-spatial mechanism in the variant renders the hydrolytic step both thermodynamically spontaneous and kinetically accessible, which providing a compelling new strategy for the efficient biodegradation of nerve agents.

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A Deep Learning-Based Framework for Valence Bond Structure Selection and Weight Prediction

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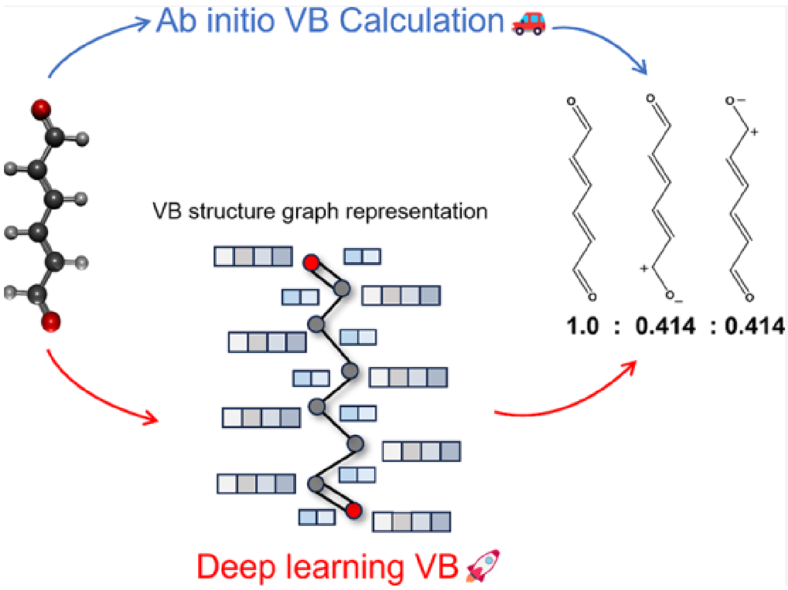
The valence bond (VB) theory offers a chemically intuitive, multiconfigurational framework for analyzing bonding, resonance, and reaction mechanisms. However, its broader application has been limited by high computational costs. In this paper, we present DLVB, a deep learning-based framework that integrates the VB theory with graph transformers through a chemically meaningful representation of VB structures. DLVB accurately predicts VB structural weights without the need for *ab initio* calculations and provides an efficient selected configuration interaction (SCI) scheme for identifying key configurations that enable the construction of compact VB wave functions. The DLVB-based SCI scheme can identify important VB structures from arbitrary structure sets within a given active space, outperforming traditional ionic-orderbased selection methods in both accuracy and scalability. This approach offers a new pathway for extending the applicability of the VB theory to the bonding analysis of systems with larger active spaces and increased molecular complexity.



Triplet-Triplet Conversion Mediated by Spin-Orbit Coupling: A Diabatic Perspective of $Ru(bpy)_3^{2+}$

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The mechanism of transitions within the triplet manifold of transition metal complexes remains elusive. While spin-orbit coupling (SOC) is essential for intersystem crossing, its potential role—likely indirect—in mediating triplet-triplet mixing is not well understood. By adopting a diabatic representation for the model system $Ru(bpy)_3^{2+}$, we decouple the complex electronic interactions to elucidate this role. Our analysis reveals that SOC does not directly cause transitions but facilitates mixing between triplet states by enabling non-adiabatic coupling. We quantify the relevant SOC matrix elements and identify the key coupling pathways. This work establishes that SOC plays a critical indirect role and provides a diabatic framework for rationally tuning photophysical properties.

Adiabatic-to-Diabatic Analysis Method for Multi-State Systems

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This work primarily focuses on an adiabatic-to-diabatic analysis method for multi-state systems. The procedure involves selecting reference states with chemical significance and constructing a weight-based objective function to quantify the similarity between the target diabatic states and the reference states. Optimizing this function determines a transformation matrix that generates diabatic states that maximally retain the chemical characteristics of the reference states. The resulting chemically intuitive diabatic states provide a robust foundation for the chemical analysis of multi-state systems.

Au[I] Complexes with Planar Tetracoordinate Carbon and Their Catalytic Activity for the Rearrangement of Allylic Acetates: A Computational Study

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Since the experimental synthesis of $C_2B_2H_2$ in 2017, the general class of $C_2B_2R_2$ with variable substituent group R has been speculated and expected. Here we computationally investigate two rhombus molecules $C_2B_2Me_2$ (**a**) and $C_2B_2tBu_2$ (**b**) which are confirmed to have carbene characteristic arising from charge shift based on the ab initio valence bond (VB) computations. These novel carbene molecules are structurally similar to N-heterocyclic carbenes (IMe and I*t*Bu). Using them as ligands, six complexes $(C_2B_2R_2)_2Au^I$, $(C_2B_2R_2)AuCl$, and $(C_2B_2R_2)Au^I$, (R=Me and *t*Bu) are designed and found to be thermodynamically stable on the basis of density functional theory (DFT) calculations. NBO analyses show that these six complexes contain planar tetracoordinate carbons (ptCs). The first vertical energies of these complexes are consistently red-shifted compared to their ligands $C_2B_2R_2$. We further explore the reaction mechanism of the rearrangement of allylic acetates catalyzed by $(C_2B_2R_2)Au^I$ (R=Me and *t*Bu) and their analogues $(NHC)Au^I$ (NHC=IMe and I*t*Bu) for comparison. It is found that the rearrangement of allylic acetates catalyzed by $(C_2B_2R_2)Au^I$ is feasible both thermodynamically and kinetically, and the concerned energy barriers in the process are lower than those catalyzed by $(NHC)Au^I$. Thus, $C_2B_2R_2$ are promising novel molecules which can be used to rationally design a variety of compounds with ptCs for potential applications in catalysis.

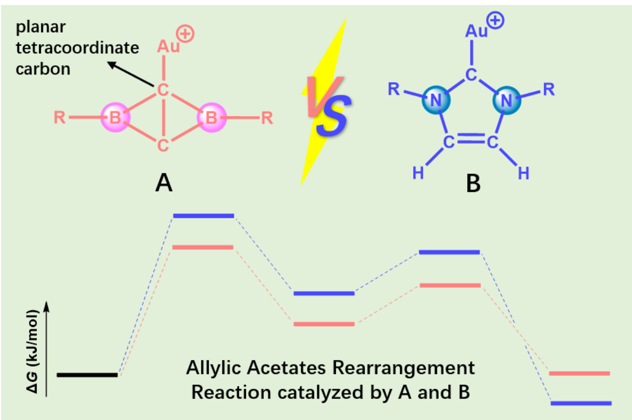

Fig. 1 Allylic Acetates Rearrangement Reaction catalyzed by A and B.

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Intermolecular Dispersion Interactions: Low-Rank Algorithms and Energy Decomposition

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Intermolecular dispersion interactions play a crucial role in various physicochemical processes. Understanding and calculating these interactions is a significant topic in theoretical chemistry. Since dispersion forces originate from electron density fluctuations in the vacuum, mean-field methods like Hartree-Fock cannot describe them. Furthermore, the high computational scaling of traditional electron correlation methods prevents their application to large systems. This work develops a tensor decomposition algorithm based on a double basis set, enabling efficient $O(N^3)$-scaling calculations for the Random Phase Approximation (RPA), GW, and Bethe-Salpeter Equation (BSE) in molecular systems. By combining this algorithm with Symmetry-Adapted Perturbation Theory (SAPT) and RPA, we have developed a method for efficiently computing and analyzing intermolecular dispersion interactions. Furthermore, to address dispersion interactions in complex environments, such as intermolecular interactions within a Fabry-Pérot optical cavity, we have developed the QED-SAPT method for treating light-matter interactions. This method can separately compute the cavity-induced R^{-3} and R^{0} terms, providing a powerful tool for understanding intermolecular interactions within optical cavities.

Keywords: Intermolecular interactions; Tensor low-rank decomposition; Electron correlation methods

Effective Two-State Model Based on Adiabatic-to-Diabatic Transformation and Its Applications

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Combining the features of the molecular orbital and valence bond theories, a novel effective two-state model based on adiabatic-to-diabatic (ATD) transformation is proposed and applied to several multistate interacting systems. This model is available not only for constructing effective diabatic wave functions but also for evaluating various diabatic properties including energy, electronic coupling, potential energy surfaces (PESs) and their crossings, etc. Moreover, in this model, the ATD transformation matrix can be deduced from the configuration interaction expansion coefficients of the adiabatic states. A series of molecules, $[NH_2{-}(CH_2)_n{-}NH_2]^+$ (n = 1-5), the hydrogen abstraction (H-abstraction) reaction and the semiglobal PESs in H_3, and the Diels−Alder reaction of 1,3-butadiene and ethylene were used as test examples to display the versatility of the model. Furthermore, the effects of electronic coupling on the barriers and the chemical reactivity of reactions in the test molecules are also discussed. Therefore, the effective two-state model can serve as a practical theoretical tool for analyzing bridge-assisted multistate electron transfer (ET) reactions and chemical reactions that involve simultaneous bond-breaking and bond-making.

MOKIT: An Open-Source Framework for Interoperability Among Quantum Chemistry Packages

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MOKIT (https://gitlab.com/jxzou/mokit) is an open-source toolkit which features data interconversion, data reuse, and interoperability among a dozen of quantum chemistry software packages. By using abundant utilities of MOKIT, one can perform an advanced ab initio calculation with each step assigned to a quantum chemistry program playing to its strengths. For example, a CASPT2 calculation from scratch can be partitioned into the HF calculation in Gaussian, orbital localization in MOKIT, GVB in GAMESS, CASSCF in PySCF, and finally CASPT2 in Molpro. Basis set (and ECP) data and molecular orbitals (MOs) are correctly transformed along with the geometry and reused in a subsequent calculation, where iteration procedures like HF/CASSCF orbital optimizations are avoided when switching to the next program. Users can either use individual utilities or adopt built-in workflows in MOKIT to accomplish a complicated calculation. Knotty problems like SCF convergence failure as well as converging to undesired SCF solutions are tackled at their source. Advantages of existing quantum chemistry software are integrated together to perform highly-efficient computations.