PROGRAM AND ABSTRACTS

TMCQ 2023

International Workshop on New Advances in Theoretical and Computational Molecular Sciences for Complex and Quantum Processes

June 27-30, 2023

Seoul, Korea

ORGANIZED BY

YounJoon Jung (Seoul National University)

Seogjoo J. Jang (CUNY-Queens College)

HOST

Department of Chemistry, Seoul National University

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Welcoming Remarks

It is our great pleasure to welcome all of you to International Workshop on New Advances in Theoretical and Computational Molecular Sciences for Complex and Quantum Processes (TMCQ 2023) at Seoul National University in Korea. The workshop will gather internationally recognized scholars to discuss recent advances and challenging issues in theoretical and computational molecular sciences. During three days of workshop at a beautiful campus of Seoul National University, participants will enjoy close interactions and open discussions in a friendly environment.

YounJoon Jung and Seogjoo J. Jang

Introduction to TMCQ 2023

Recent advances in theories and computational methods have opened ways for successful description of various complex phenomena and quantum processes from mesoscopic scale down to molecular details. Along with experimental progresses such as nonlinear spectroscopy, high resolution imaging, and nanoscale manipulation techniques, those advances now make it possible to understand complicated molecular processes at unprecedented level of accuracy and details. Many complex phenomena and quantum processes that seemed impossible to grasp are now within the realm of quantitative description and prediction. Exemplary areas include energy/charge transfer, complex fluids, and biophysical processes ranging many orders of magnitudes both in time and length scales. However, as these research fields become highly specialized, different research communities, in particular, experts in statistical mechanics and quantum dynamics, mostly remain disjoint from each other. On the other hand, new and challenging theoretical and computational issues to be addressed in complex and quantum mechanical phenomena such as polaritonics, plasmonics, quantum sensing, and energy sciences call for integration and crosscutting of different research areas more than ever. Another key factor to consider is the accelerating progress in machine learning approaches, which may have a potential of fundamentally transforming theoretical and computational molecular sciences. During the workshop we will discuss recent advances in theories and methodologies in these fields to assess outstanding issues to be resolved.

Program at a Glance

June 27 (Tue)	**June 28 (Wed)**		**June 29 (Thu)**		**June 30 (Fri)**	
Cherry Room, Hoam Main Bldg.	**Mogam Hall, Chemistry Dept.**		**Rose Room, Hoam SK Guest House**		**Rose Room, Hoam SK Guest House**	
6:30 Reception/ Dinner	**Session 1: S. J. Jang**		**Session 5: C. H. Choi**		**Session 9: C. Y. Son**	
	9:30 -10:10	E. Pollak	9:30 -10:10	J. Cao	9:00 -9:40	S. Flach
	10:10 -10:50	C. H. Choi	10:10 -10:50	S. J. Jang	9:40 -10:20	J. Sung
	10:50 -11:10	Coffee Break	10:50 -11:10	Coffee Break	10:20 -10:40	Coffee Break
	Session 2: C. Hyeon		**Session 6: B. J. Sung**		**Session 10: J. S. Kim**	
	11:10 -11:50	M. E. Tuckerman	11:10 -11:50	F. L. H. Brown	10:40 -11:20	Y. Jung
	11:50 -12:30	T. Bereau	11:50 -12:30	C. Hyeon	11:20 -11:50	C. Y. Son
	12:30 -14:00	Lunch	12:30 -14:00	Lunch	12:00 -13:00	Lunch
	Session 3: S. K. Min		**Session 7: C. W. Myung**		13:00	Excursion
	14:00 -14:40	O. V. Prezhdo	14:00 -14:40	F. Paesani		
	14:40 -15:20	Y. M. Rhee	14:40 -15:20	C.-P. Hsu		
	15:20 -15:40	Coffee Break	15:20 -15:40	Coffee Break		
	Session 4: Y. M. Rhee		**Session 8: Y. Jung**			
	15:40 -16:10	S. Ringe	15:40 -15:20	J. S. Kim		
	16:10 -16:40	C. W. Myung	16:20 -17:00	B. J. Sung		
	16:40 -16:50	Group Photo	17:00 -17:20	Coffee Break		
	Poster Session		17:20 -18:00	S. K. Min		
	16:50 -18:20	Poster Session				
	18:30	Dinner	18:30	Banquet (Rose Rm.)		

PROGRAM

June 28 (Wed)
Mogam Hall, Chemistry Department

Session 1: Seogjoo J. Jang (CUNY-Queens)

9:00 - 9:25		Registration
9:25 - 9:30	Seogjoo J. Jang (CUNY-Queens)	Opening and Introductory Remarks
9:30 - 10:10	Eli Pollak (Weizmann Institute)	Some Observations on Quantum Thermal Rate Theory
10:10 - 10:50	Cheol Ho Choi (Kyungpook Nat'l Univ.)	MRSF-TDDFT: A Simple Yet Powerful Tool
10:50 - 11:10		Coffee Break

Session 2: Changbong Hyeon (KIAS)

11:10 - 11:50	Mark E. Tuckerman (New York Univ.)	Synergizing Enhances Sampling and Machine Learning Strategies for Finding Reaction Coordinates of Complex Processes
11:50 - 12:30	Tristan Bereau (Univ. of Heidelberg)	The Role of Coarse-Graining in Molecular Discovery

12:30 - 14:00		Lunch

Session 3: Seung Kyu Min (UNIST)

14:00 - 14:40	Oleg V. Prezhdo (Univ. of Southern California)	Ab Initio Quantum Dynamics of Nanoscale Materials for Energy and Optoelectronic Applications
14:40 - 15:20	Young Min Rhee (KAIST)	Early Stage Photodynamics of Photoactive Yellow Protein Simulated with the Interpolated Mechanics/Molecular Mechanics (IM/MM) Method
15:20 - 15:40		Coffee Break

Session 4: Young Min Rhee (KAIST)

15:40 - 16:10	Stefan Ringe (Korea Univ.)	Computationally Facilitated Screening and Understanding of Electrochemical CO_2 Reduction Catalysts
16:10 - 16:40	Chang Woo Myung (Sungkyunkwan Univ.)	Development of Next Generation Sparse Gaussian ab initio Machine Learning Potential
16:40 - 16:50		Group Photo

16:50 - 18:20		**Poster Session**
18:30		Dinner

June 29 (Thu)
Rose Room, Hoam SK Guest House

Session 5: Cheol Ho Choi (Kyungpook Nat’l Univ.)

9:25 - 9:30	Seokmin Shin (Seoul Nat’l Univ.)	Welcoming Remarks
9:30 - 10:10	Jianshu Cao (MIT)	Quantum Diffusion in Organic Materials: Disorder, Phonons, and Photons
10:10 - 10:50	Seogjoo J. Jang (CUNY-Queens)	Exciton and Charge Transfer Theories Based on Fermi’s Golden Rule and Beyond
10:50 - 11:10	Coffee Break	

Session 6: Bong June Sung (Sogang Univ.)

11:10 - 11:50	Frank L. H. Brown (UC Santa Barbara)	Correlated Diffusion in Lipid Bilayer Membranes
11:50 - 12:30	Changbong Hyeon (KIAS)	Irregularity of Polymer Domain Boundaries in Two-dimensional Polymer Solution
12:30 - 14:00	Lunch	

Session 7: Chang Woo Myung (Sungkyunkwan Univ.)

14:00 - 14:40	Francesco Paesani (UC San Diego)	Data-Driven Many-Body Potentials for Realistic Molecular Simulations of Aqueous Systems and Beyond
14:40 - 15:20	Chao-Ping Hsu (Academia Sinica)	Dynamic Disorder of Nonpolar Systems with Machine-learned Electron Transfer Coupling
15:20 - 15:40	Coffee Break	

Session 8: YounJoon Jung (Seoul Nat’l Univ.)

15:40 - 16:20	Jun Soo Kim (Ewha Womans Univ.)	Brownian Ratchet for Directional Molecular Transport by Stimuli-responsive, Repetitive Aggregations and Dispersion
16:20 - 17:00	Bong June Sung (Sogang Univ.)	A Molecular Simulation Study for the Packaging and the Ejection Processes of Viral DNA
17:00 - 17:20	Coffee Break	
17:20 - 18:00	Seung Kyu Min (UNIST)	Correlated Electron-Nuclear Dynamics Toward Extended Systems
18:30	Banquet	

June 30 (Fri)
Rose Room, Hoam SK Guest House

Session 9: Chang Yun Son (POSTECH)

9:00 - 9:40	Sergej Flach (IBS-PCS)	Flat Band Induced Metal-Insulator Transitions
9:40 - 10:20	Jaeyoung Sung (Chung-Ang Univ.)	Nonclassical Dynamics of Chemical and Transport Processes in Living Cells and Nanomaterial Systems
10:20 - 10:40	Coffee Break	

Session 10: Jun Soo Kim (Ewha Womans Univ.)

10:40 - 11:20	YounJoon Jung (Seoul Nat'l Univ.)	Exploring Free Energy Profiles in and Far from Equilibrium
11:20 - 11:50	Chang Yun Son (POSTECH)	Universal Dipole Correlation in Homogeneous Bulk and Interfacial Water
11:50 - 11:55	YounJoon Jung (Seoul Nat'l Univ.)	Closing Remarks
12:00 - 13:00		Lunch
13:00	Excursion	

ABSTRACTS OF TALKS

S1-1

Some Observations on Quantum Thermal Rate Theory

Eli Pollak

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There are a number of aspects of reactive collisions and rate theory which have eluded researchers. The first to be addressed in an $\hbar^2$ expansion of the thermal rate. Ninety years ago, Wigner derived the leading order term for symmetric reactions. The full expression valid for asymmetric reactions and including terms up to order $\hbar^4$ has been derived only very recently [1]. The resulting expression will be presented and discussed, especially in the view of challenging existing approximate theories which reduce to the parabolic barrier expression but do not account correctly for anharmonic effects. One aspect which emerges from these investigations is that above barrier quantum reflection may reduce the quantum thermal rate as compared with the classical rate.

The same result will then be used within the context of a recently formulated coherent state phase space representation of operators used to derive an exact expression for the symmetrized version of thermal correlation functions and especially the flux side correlation function which is used to obtain reaction rates. [2] The coherent state representation necessitates the use of a smeared Gaussian flux operator, whose coherent state phase space representation is identical to the classical flux expression. The resulting coherent state expression provides a route for analytic semiclassical approximations for the thermal rate, as exemplified by a computation of the transmission factor through a symmetric and an asymmetric Eckart barrier using a thawed Gaussian approximation for both imaginary and real-time propagation. As a byproduct, this example shows that one may obtain "good" tunneling rates using only above barrier classical trajectories even in the deep tunneling regime. [3]

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S1-2

MRSF-TDDFT: A Simple Yet Powerful Tool

Seunghoon Lee, Woojin Park, Hiroya Nakata, Konstantin Komarov, Toby Zeng, Miquel Huix-Rotllant, Michael Filatov, Cheol Ho Choi

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A new quantum theory, MRSF-TDDFT (Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory) has been developed for both ground and excited electronic states. With the help of a unique spinor-like transformation, a *hypothetical* single reference is constructed from the two M_S = +1 and -1 components of the RO-KS determinant, which makes the equal-ensemble density idempotent for the linear-response formalism.

As a result, MRSF-TDDFT

(a) is equipped with both *dynamic* and *nondynamic* (including doubles) electron correlation,
(b) eliminates the spin-contaminations of SF-TDDFT,
(c) produces correct topology of conical intersection,
(d) allows to study bond-breaking as well as open-shell singlets such as diradicals,
(e) but still has $O(N^4)$ scaling with the convenience of single determinant orbital optimization.

Now the theory is combined with NAMD, QM/MM, Relativistic effects, and Extended Koopman Theorem. Here, we highlight its advantages and promising performances by presenting our recent results on Jahn-Teller distortions, excited state nonadiabatic dynamics, conical intersection, open shell singlet system, nonadiabatic coupling, spin-orbit coupling and X-ray absorption/ionization applications.

References

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(c) Park, W., Shen, J., Lee, S.; Piecuch, P., Filatov, M., Choi, C. H. (**2021**) *J. Phys. Chem. Lett.*, 12, 39, 9720–9729,

S2-1

Synergizing Enhanced Sampling and Machine Learning Strategies for Finding Reactions Coordinates of Complex Processes

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Machine learning has become an integral tool in the theoretical and computational molecular sciences. Uses of machine learning in this area include prediction of molecule and materials properties from large databases of descriptors, design of new molecules with desired characteristics, design of chemical reactions and processes, representation of high-dimensional potential energy and free energy surfaces, creation of new enhanced sampling strategies, and bypassing of costly quantum chemical calculations, to highlight just a few. This lecture will focus on the use of machine learning and rare-event sampling strategies for finding reaction coordinates that characterize transitions between different basins on high-dimensional free energy surfaces and generating pathways between these basins. We will first review collective-variable based enhanced sampling techniques and then compare different classes of machine learning models, including kernel methods, neural networks, decision-tree approaches, and nearest-neighbor schemes for performing the aforementioned tasks. Specific examples from materials science and biomolecules will be used to illustrate the synergistic schemes.

S2-2

The Role of Coarse-Graining in Molecular Discovery

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Advanced statistical methods are rapidly impregnating many scientific fields, offering new perspectives on long-standing problems. In materials science, data-driven methods are already bearing fruit in various disciplines, such as hard condensed matter or inorganic chemistry, while significantly less has happened in soft matter. I will describe how we use multiscale simulations to leverage data-driven methods in soft matter. We aim at establishing structure-property relationships for complex thermodynamic processes across the chemical space of small molecules. Akin to screening experiments, we devise a high-throughput coarse-grained simulation framework. Coarse-graining is an appealing screening strategy for two main reasons: it significantly reduces the size of chemical space and it helps suggest a low-dimensional representation of the structure-property relationship. To illustrate these aspects, I will focus on a complex biomolecular system: the selective binding of small molecules to cardiolipin in mitochondrial membranes. A multiscale compound search helps us identify clear design rules for highly selective molecules. It also eases the identification of compounds for experimentation in vitro and in vivo.

S3-1

Ab Initio Quantum Dynamics of Nanoscale Materials for Energy and Optoelectronic Applications

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Excited state dynamics play key roles in numerous molecular and nanoscale materials designed for solar energy conversion and optoelectronic devices. Controlling these far-from-equilibrium processes and steering them in desired directions require understanding of material's dynamical response on the nanometer scale and with fine time resolution. We couple real-time time-dependent density functional theory for the evolution of electrons with non-adiabatic molecular dynamics for atomic motions to model such non-equilibrium response in the time-domain and at the atomistic level. The talk will introduce the simulation methodology [1] and discuss several exciting applications among the broad variety of systems and processes studied in our group [2,3], including metal halide perovskites, transition metal dichalcogenides, semiconducting and metallic quantum dots, metallic and semiconducting films, polymers, molecular crystals, graphene, carbon nanotubes, etc. Photo-induced charge and energy transfer, plasmonic excitations, Auger-type processes, energy losses and charge recombination create many challenges due to qualitative differences between molecular and periodic, and organic and inorganic matter. Our simulations provide a unifying description of quantum dynamics on the nanoscale, characterize the timescales and branching ratios of competing processes, resolve debated issues, and generate theoretical guidelines for development of novel systems.

References

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S3-2

Early Stage Photodynamics of Photoactive Yellow Protein Simulated with the Interpolated Mechanics / Molecular Mechanics (IM/MM) Method

Young Min Rhee

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Simulating photodynamics of any protein system involves somehow building the potential energy surfaces (PES's) of multiple electronic states together with their coupling elements. Building models for such PES's is never a trivial task and QM/MM often becomes the method of choice as it can avoid the headaches of modeling. Practically, however, reaching statistical certainty with enough number of trajectories with QM/MM is also non-trivial especially with a large protein complex. The interpolation mechanics / molecular mechanics (IM/MM) has been designed as a remedy, toward reaching this certainty without sacrificing the reliability. Here, we will discuss how the IM/MM surface construction is attained for the photoactive yellow protein (PYP) complex. We will focus on the aspect of fine-tuning the interface area between the IM and the MM regions. With actual dynamics simulations, we will demonstrate that the constructed PES can be utilized for obtaining thousands of nonadiabatic surface hopping trajectories into a timescale of a nanosecond. We will attempt to explain the peculiarities of PYP dynamics based on the simulated trajectories.

S4-1

Computationally Facilitated Screening and Understanding of Electrochemical CO_2 Reduction Catalysts

Stefan Ringe

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Electrochemical CO_2 reduction is at the heart of the world's effort toward a sustainable energy future. Despite this, devices have not yet been optimized to the performance level needed to overthrow conventional thermochemical processes. Computational quantum chemical simulations can help to get a deep understanding of the working principle and stability of these catalysts, and also to perform high-throughput screening of suitable materials. In this talk, I first introduce a computational method based on density functional theory which accounts for the electric double layer essential for many electrochemical reactions. From this, I derive a methodology and descriptor space for screening suitable electrocatalysts for CO_2 reduction. Finally, examples are presented of how computational tools can be used to deeply understand complex materials such as ceria under electrochemical conditions.

S4-2

Development of Next Generation Sparse Gaussian Ab Initio Machine Learning Potential

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In recent years, machine learning has transformed numerous scientific disciplines by tackling key challenges. Machine learning potentials offer a promising avenue for surmounting the stringent limitations on size and speed, which are inherent to ab initio simulations [1]. We develop the transferable sparse Gaussian process regression (SGPR) machine learning potential, which scales linearly O(n) by leveraging active inducing selection techniques [2,3,4,5]. By taking advantage of the kernel structure, the SGPR machine learning potential can be expanded into a general potential for all known compounds. The SGPR machine learning potential has been developed for a variety of materials, including Li solid electrolytes [2], hydrocarbons [3], Li-battery cathodes [4], and aqueous solutions [5]. Presently, machine learning potentials only predict ab initio energy based on geometric information, which lacks crucial electronic details such as charge states, excited states, and spin interactions. To address this limitation, we incorporate the missing electronic structure information, including electron transfer [5] and spin-spin interactions [6], enhancing its predictive capabilities of the SGPR potential. The ultimate goal is to build and apply this general-purpose ab initio machine learning potential to investigate various complex reactions such as catalysis, electron transfer, protein folding, and adsorption phenomena on surfaces.

References

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S5-1

Quantum Diffusion in Organic Materials: Disorder, Phonons, and Photons

Jianshu Cao

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In the first part of the talk, I will present calculations of coherent charge and exciton transport in disordered systems, which reveal an optimal diffusion constant at the crossover between the coherent and incoherent regimes.[1] The quantum enhancement in the coherent regime depends on the dimension and shape of the sample and exhibits a universal scaling.[2] Mapping of quantum to kinetic networks provide both an intuitive understanding of these coherent features and a potentially useful numerical technique. Though transport is suppressed by disorder, trapping or dissociation can be enhanced by disorder.[3]

In the second part of the talk, I will discuss recent results on quantum diffusion assisted by phonons or cavity photons. Our analysis of the tilted Holstein model predicts the fractional vibronic resonance, which is supported by mapping the Holstein model to a continuous time random walk.[4] In optical cavities, disordered molecules are coupled to cavity fields collectively, such that the cooperativity in the light-matter interaction can overcome the Anderson disorder and lead to a turnover in transport at an optimal level of static disorder.[5]

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S5-2

Exciton and Charge Transfer Theories Based on Fermi's Golden Rule and Beyond

Seogjoo J. Jang

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For the development and refinement of novel solar light harvesting, energy storage, and quantum sensing devices, efficient and accurate computational methods to describe and model the quantum transfer/transport of excitons and charge carriers in complex and confined molecular environments play crucial roles. Although significant advances have been made in theories and computational methods of quantum dynamics in recent years, simple theories based on Fermi's golden rule (FGR) still remain some of the most widely used theories that are conceptually clear and reasonably accurate for describing quantum transitions in complex systems with significant disorder/fluctuations. In this talk, I will provide a short summary of FGR-based generalizations of Förster resonance energy transfer theory, Electron transfer theory, and the energy gap law that I have developed to account for various quantum effects at minimal computational costs. Applications of some of these to light harvesting complexes and organic molecular aggregates are demonstrated as well. Then, I will introduce ongoing theoretical efforts to go beyond simple rate description through generalized master equation, quantum master equation, and quantum Fokker-Planck equation approaches.

S6-1

Correlated Diffusion in Lipid Bilayer Membranes

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Dual-color single-molecule tracking can directly measure dynamic lipid-lipid correlations in membranes. Unfortunately, quantitative interpretation of these measurements is not entirely straightforward, due to both the inhomogeneous hydrodynamic environment (two opposing lipid monolayers embedded in an aqueous bulk) and finite acquisition times associated with experiment. I will discuss both the experiments carried out by my collaborators (Rafael Schoch and Gilad Haran) and the theoretical interpretation of them.

S6-2

Irregularity of Polymer Domain Boundaries in Two-Dimensional Polymer Solution

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Polymer chains comprising a polymer solution in strict two dimensions (2D) are characterized with irregular domain boundaries, whose fractal dimension (D^{∂}) varies with the area fraction of the solution and the solvent quality. We find that D^{∂} in good solvents changes non-monotonically from $D^{\partial} = 4/3$ in dilute phase to $D^{\partial} = 5/4$ in dense phase, maximizing to $D^{\partial} \approx 3/2$ at a critical area fraction, whereas for polymers in Θ solvents D^{∂} remains constant at $D^{\partial} = 4/3$ from dilute to semi-dilute phase. Using polymer physics arguments, we rationalize these values, and show that the maximum irregularity of $D^{\partial} \approx 3/2$ is due to “fjord"-like corrugations formed along the domain boundaries which also maximize at the same critical area fraction. Our finding of $D^{\partial} \approx 3/2$ is, in fact, in perfect agreement with the upper bound for the fractal dimension of the external perimeter of 2D random curves at scaling limit, which is predicted by the Schramm-Loewner evolution (SLE).

S7-1

Data-Driven Many-Body Potentials for Realistic Molecular Simulations of Aqueous Systems and Beyond

Francesco Paesani

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Two of the most challenging problems at the intersection of electronic structure theory and molecular dynamics simulations are the accurate representation of intermolecular interactions and the development of efficient algorithms applicable to large systems. To some extent, these two problems are antithetical, since accurate calculations of molecular interactions typically require correlated electronic structure methods that are computationally too expensive for applications to large systems. In my talk, I will describe our data-driven many-body energy (MB-nrg) formalism, which overcomes these limitations and enables realistic computer simulations from the gas to the condensed phase. MB-nrg is a unified theoretical/computational framework that integrates data-driven machine-learned representations of individual many-body interactions with physics-based (mean-field-like) many-body models. I will illustrate the accuracy, transferability, and predictive power of our MB-nrg potentials for various molecular systems, from gas-phase clusters to bulk solutions, interfaces, and porous materials.

S7-2

Dynamic Disorder of Nonpolar Systems with Machine-Learned Electron Transfer Coupling

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Electron transfer (ET) is a fundamental process in chemistry and biochemistry, and electronic coupling is an important determinant of the rate of ET. However, electronic coupling is sensitive to many nuclear degrees of freedom, particularly those involved in intermolecular movements, making its characterization challenging. As a result, dynamic disorder in electron transfer coupling has rarely been investigated, hindering our understanding of charge transport dynamics in complex chemical and biological systems. We have developed machine-learning models[1,2] for ET couplings, and its dynamic disorder in coupling can be studied. For nonpolar model systems, ethylene and napathalene, our results reveal that low-frequency modes dominate these dynamics, resulting primarily from intermolecular movements such as rotation and translation, with sub-Ohmic character, with cut-off frequencies in the range of 10^2 cm^{-1}.

References

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S8-1

Brownian Ratchet for Directional Molecular Transport by Stimuli-Responsive, Repetitive Aggregation and Dispersion

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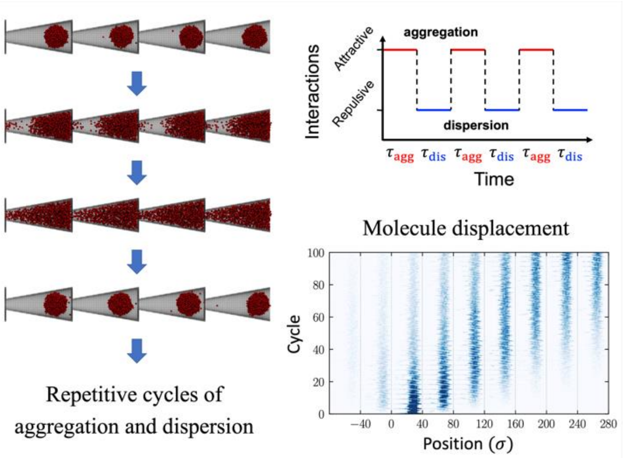
We propose a Brownian ratchet mechanism for the unidirectional transport of stimuli-responsive molecules confined in a series of asymmetric geometries. This mechanism relies on repetitive cycles of aggregation and dispersion, which cause significant changes in molecular distribution within the confining geometry and enable molecular motions to be ratcheted in a specific direction. It can be effective even for small molecules, overcoming the size limit of earlier Brownian ratchet mechanisms. To demonstrate the feasibility of this mechanism, we conducted Brownian dynamics (BD) simulations where molecules in Brownian motion were repetitively aggregated and dispersed in a series of truncated conical tubes by altering intermolecular interactions to mimic the effect of external stimuli. Our simulations demonstrated the unidirectional transport of the molecules, indicating the efficacy of the proposed mechanism. Furthermore, we found that the mechanism becomes more effective with higher concentrations of molecules. This study suggests that the precise design of stimuli-responsive molecular interactions can be used for directional and controlled molecular transport in nanoscale applications.



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A Molecular Simulation Study for the Packaging and the Ejection Processes of Viral DNA

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DNAs are packaged into and ejected from a small viral capsid during the virus replication process. Single molecule experiments were performed to understand how the DNA could overcome a large entropy loss and a strong pressure during packaging. Theoretical studies also reported how the DNA was jammed in non-equilibrium states inside the capsid. It is also an issue how such non-equilibrium jammed conformation would affect the DNA ejection from a viral capsid. Unfortunately, however, packaging and ejection processes have been treated as independent processes under the assumption that the DNA would reach an equilibrium conformation. In this presentation, I would like to report that the ejection process of DNA from the viral capsid should depend significantly on how the DNA was packaged into the viral capsid. We perform Langevin dynamics simulation to package the DNA into a viral capsid and let the DNA eject from the capsid spontaneously. There should be three different regimes depending on the packaging rate: (1) knot dominant, (2) non-equilibrium dominant, and (3) intermediate regimes. When the DNA is packaged slowly, the DNA forms a complex knot easily during the packaging such that the ejection slows down (knot dominant regime). When the DNA is packaged quickly, the DNA is more likely to be jammed in non-equilibrium states, slowing down the ejection process (non-equilibrium dominant regime). When the packaging rate is intermediate, the probability of knot conformation is relatively low, and the DNA conformation may also relax easily, which facilitate the ejection most (intermediate regime).

S8-3

Correlated Electron-Nuclear Dynamics Toward Extended Systems

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Correlated electron-nuclear dynamics is crucial in various phenomena, including photosynthesis, photovoltaics, photocatalysis, radiation chemistry, polaron chemistry, and quantum computing. Electron-nuclear correlations are handled using mixed quantum-classical approaches for small and intermediate molecular systems.[1] However, for extended molecular systems, real-time time-dependent density functional theory (RT-TDDFT) is used frequently. RT-TDDFT propagates electronic density with time-dependent Kohn-Sham orbitals and time-dependent external potentials while the classical nuclei move according to the Ehrenfest-type equation of motion. While the electronic equation of motion can describe nonadiabatic transitions, it cannot account for nuclear wave packet splitting and quantum decoherence, which are crucial for describing long-time behavior. To overcome this limitation, we propose a Hermitian form of an electron-nuclear correlation operator, which is equivalent to the original non-Hermitian operator.[2] This approach obtains a stable real-time and real-space electronic propagation with quantum decoherence in correlated electron-nuclear dynamics, which is essential for condensed phase simulations. Furthermore, we devise a modified version of the time-dependent Kohn-Sham equation by employing a Hermitian correlation operator within the RT-TDDFT framework. The approach is demonstrated to work well for molecular and condensed matter systems. The proposed method may pave the way for using the RT-TDDFT framework with the electron-nuclear correlation from the exact factorization approach for the simulation of extended systems for material science applications where a large number of electronic BO states are involved in the dynamics.

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S9-1

Flat Band Induced Metal-Insulator Transitions

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Certain lattice wave systems in translationally invariant settings have one or more spectral bands that are strictly *flat* or independent of momentum in the tight binding approximation, arising from either internal symmetries or fine-tuned coupling [1]. Originally considered as a theoretical convenience useful for obtaining exact analytical solutions of ferromagnetism, flat bands have now been observed in a variety of settings, ranging from electronic systems to ultracold atomic gases and photonic devices [1],[2]. I will review the design and implementation of flat bands, classification schemes, discuss recent results on adding many-body interactions [3] and disorder [4], and chart future directions of this exciting field.

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S9-2

Nonclassical Dynamics of Chemical and Transport Processes in Living Cells and Nanomaterial Systems

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We will present a new theoretical approach for effective, quantitative description of complex dynamical processes and their networks in living cells and nanomaterial systems. In doing so, we will introduce our new models and theories on chemical dynamics and transport dynamics in these systems. Particularly we will talk about the recently proposed transport equation governing stochastic thermal motion of complex fluids and the chemical fluctuation theorem that links the mean and fluctuations of mRNA and protein concentrations to the gene regulation mechanism and dynamics of elementary processes constituting the gene network. We will demonstrate successful applications of these theories and their recent generalizations for quantitative understanding of signal propagation and signal-induced gene expression dynamic in living cells. We will also briefly discuss the thermodynamic origin of nucleus seed formation and their nonclassical growth dynamics.

S10-1

Exploring Free Energy Profiles in and Far from Equilibrium

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We discuss our recent studies on exploring free energy profiles, both in and out-of-equilibrium situations. As an out-of-equilibrium case, we introduce trajectory ensemble approach to dynamical phase transitions in complex systems. As prototypical example, we investigate the dynamical phase transition behavior of the one-dimensional Ising model. We introduce a novel, double-biased ensemble, named *s, g*-ensemble, based on non-equilibrium steady-state trajectories. Within the ensemble, the dynamical free energy is analytically available, which allows us to explore the rich behaviors of the dynamical phase transition of the system in details. While the equilibrium phase diagram of the 1D Ising model is mundane, we reveal that novel, anomalous dynamical phase transitions are possible due to the decoupling between the dynamical activity and trajectory energy under specific conditions. In particular, we observe that the system exhibits a freezing-by-heating phenomenon as the dynamical activity decreases with temperature under a specific condition. We also find a permanent liquid phase when the equilibrium temperature and the non-equilibrium *g*-field are exactly balanced against each other. Applications of the approach to other systems are currently underway.

In the second case, we present a novel, computationally efficient yet accurate strategy to explore the free energy landscapes of chemical reactions at atomistic level. Our approach combines single point DFT calculations and well-tempered metadynamics method, augmented by a free energy perturbation scheme and deep-learning estimator for the single-point energetics. The approach alleviates the need to perform high-level DFT MD calculation for an efficient sampling of the free energy surface. We illustrate our approach using the example of Diels-Alder reaction with post-transition state bifurcation, and obtain a free energy surface that is in quantitative agreement with transition state theory calculations. In this system, two major reaction pathways are analyzed in detail with appropriately chosen CVs. Our general approach can be applied to complex chemical reactions.

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S10-2

Universal Dipole Correlation in Homogeneous Bulk and Interfacial Water

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Understanding electrostatic interactions near surfaces and interfaces is of critical importance in various fields of science. The interplay of electrostatic interactions through the symmetry-breaking boundaries plays the major role in thermodynamic and dynamic behavior of the system. Recent advances in surface specific spectroscopic techniques have greatly enhanced our understanding on these interfacial phenomena, although precise molecular understanding of these complex systems is still challenging. Strong confinement induced by two of such dielectric interfaces provide unique environment for novel materials synthesis and manipulation.

This study investigates the anomalous behavior observed in strongly confined water, specifically the significant reduction in its dielectric constant that has been confirmed through experimental and simulation studies. Using molecular dynamics simulations that fully incorporate the dielectric response of confining walls, we aimed to identify the molecular mechanisms governing the dielectric reduction. Our simulations revealed that the reduction in dielectric constant occurs independently of the electronic polarization at the surface, which contradicts previously proposed mechanisms. We also found that the local fluctuation in the dipole of a water slab does not vary significantly from the locally aligned interfacial region to the homogeneous bulk region. Instead, we discovered that a small, positive dipolar correlation between a set of water slabs plays a critical role in determining the total dielectric response of the confined water. We found that the long-range correlation is independent of the confinement size and the interfacial structure, resulting in a linear correspondence between the confinement length and the total dielectric constant in the direction orthogonal to the confining wall surface. Furthermore, our simulation suggests that allowing capillary fluctuation on the interfacial water structure mitigates the dielectric reduction. Our findings provide novel insights into the nature of the observed anomalous behavior and have important implications for controlling and designing interfacial electrochemical systems.

ABSTRACTS OF POSTERS

P1

Constructing Neural Network Potentials for TiN-ALD Process Simulations

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Surface reactions such as atomic layer deposition (ALD) play a crucial role in the semiconductor industry. Traditional density functional theory methods, while effective, can be computationally intense and time-consuming, especially when observing rare events in molecular dynamics. Neural network potentials (NNP) offer a more efficient alternative, capable of rapidly predicting atomic structure energy and forces with high accuracy. However, developing the appropriate training set for NNP can be challenging, particularly when detailed knowledge of the reaction mechanism is lacking. In this study, we address this challenge using an active-learning method combined with single-ended saddle point search. We apply this approach to the TiN-ALD process, utilizing $TiCl_4$ and NH_3 as precursors. We repeatedly search for reaction mechanisms to test the robustness of our NNP. We then examine the TiN-ALD growth process and compare our findings with previous research, using our NNP to simulate growth behavior and observe the surface of TiN thin films. Our primary objective is to present a robust and straightforward method for developing NNPs, particularly in cases where knowledge about surface reactions is limited. This novel method offers a potential to expedite process simulations and enhance our understanding of surface reactions.

Development of Efficient Saddle Points Searching Methods: Application on Oxidized Platinum Surface with machine-learned potentials

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Atomistic modeling has significantly contributed to our scientific knowledge over the past several decades, delivering a detailed information of chemical processes at atomic level. However, many chemical processes have a long temporal scale that is beyond the capabilities of conventional approaches such as density functional theory (DFT) calculations and classical molecular dynamics (MD) simulations. On the other hand, kinetic Monte Carlo (kMC) simulations can investigate long-term evolution, using an event table to transition between local minima. To build the event table on-the-fly, kMC simulation needs an efficient algorithm that identifies saddle points in open-ended style.

In this study, we will discuss the results of exhaustive reactions searching on a 2 nm × 2 nm Pt(111) surface. First, for accelerated computation, we employ Behler-Parinello type machine-learned potentials (MLPs) as surrogate models of DFT. The present MLP showed energy and force root-mean-square errors of 7 meV/atom and 0.22 eV/Å, respectively, on the DFT validation set. The validation set consists of platinum oxide phases and randomly scattered oxygen atoms on platinum surface. Next, we found that the even state-of-the-art algorithm, such as ARTn, has difficulties in identifying saddle points due to the presence of soft modes prevailing on the surface. To address this, we developed the SHERPA (Saddle point Hunting based on Energy surface for Reaction PAthways) package, integrating two key features: constrained-orthogonal relaxation within ARTn and dynamic-active volume. These improvements resulted in a 30% higher success ratio and reduced computational time compared to the conventional ARTn algorithm. Even with additional constraints, SHERPA successfully found all *a priori* expected reactions. We believe this study not just enhances the efficiency of saddle points searching algorithm, but also paves the way to on-the-fly kMC simulation.

P3

Modeling Charge Transport in OLED Materials Using Multiscale Computational Chemistry Methodology

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OLED displays have gained significant attention in the display industry. Despite their popularity, OLED displays still have several challenges to overcome, particularly their short lifetime, especially in the blue color diodes. In general, OLED material research employs a screening method involving the synthesis of numerous candidate materials, followed by an analysis to identify suitable molecules. However, this approach is time-consuming and demanding. The in-silico approach not only provides a viable alternative, but also offers a new perspective for exploring properties from a microscopic point of view. The simulation of OLED materials requires simulations over a broad range of length and timescales. In this study, we employed the molecular dynamics technique to acquire the amorphous structure of OLED materials. Subsequently, we conducted DFT calculations for each neighboring pairs to calculate the site energy difference and transfer integral. The hopping rate of the charge carrier between molecules was obtained using semiclassical Marcus Theory, and kinetic Monte Carlo simulations were performed based on this rate to determine the charge carrier mobility. For several materials, we achieved mobility values that are close to reference experimental values.

P4

Diffusiophoretic Flows in Microchannels Studied by a Coupled Method of Molecular Dynamics and Multiparticle Collision Dynamics

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Diffusiophoretic flow is main mechanism of molecule motors or nano-motors. We study the diffusiophoretic flow using a coupled method of multiparticle collision dynamics and molecular dynamics. The proper boundary condition algorithm is introduced to make a no-slip hydrodynamic boundary condition. The pressure-driven flow is simulated to check the validity of the coupled method. In a steady-state concentration gradient, diffusiophoretic fluid flows are created along the channel. A different concentration gradient is observed near the surface than bulk liquid. This difference induces a unique flow pattern. We observe the unique flow pattern and compare the flow velocities to the theoretical values.

P5

Quantitative Estimation of Conformation and Substituent Effects on the Efficiency of Photochemical Ring-Opening

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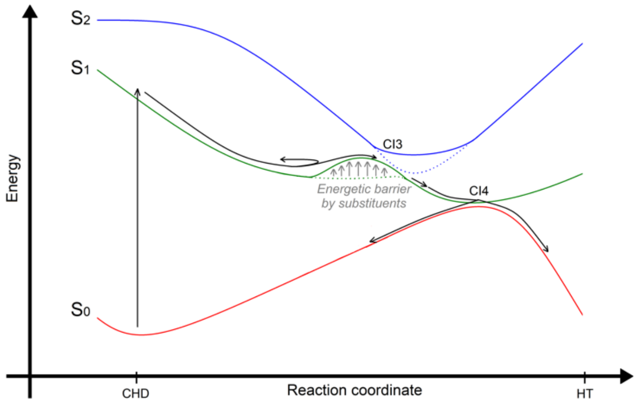
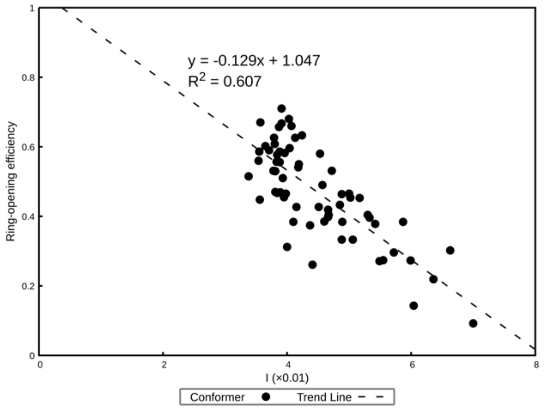
Photochemical ring-opening reactions are one of the most extensively employed chemical reactions in the field of chemistry. Owing to their significance, they have been widely studied using both theoretical and experimental approaches. However, until now, many of studies dealing with this at the molecular scale have been for the simplest one: ring-opening of 1,3-cyclohexadiene to 1,3,5-hexatriene. Recently, research on more complex cases have been conducted and it has been reported that the dynamics are affected by the substituent and conformation of the molecule, but they have been limited to one specific molecule. This implies that a law for measuring the effect of molecular structure, such as substituents and conformations, on the photochemical ring-opening in general cases has not been known. Here, we propose a hypothetic concept as a candidate of this general rule, termed 'substituent-induced electron density leakage'. Based on our hypothesis, we present an indicator which can predict the efficiency of photochemical ring-opening reactions of various conformers. Relative error between the ring-opening efficiency obtained from nonadiabatic simulations and the one obtained from the indicator introduced here was less than 25% in 56 out of 66 conformers arise from 1,3-cyclohexadiene and 12 distinct kinds of its analogs. This offers a possibility of accurately and quickly predicting the photochemical ring-opening efficiency of arbitrary molecules in arbitrary conformation.





P6

Deciphering the Mechanisms of Cholesterol Transport in the Human Body : Molecular Dynamics Simulations Study

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Our body relies on cholesterol for various essential functions, including its role as a component of biological membranes, a precursor for steroidal hormones, and a ligand for multiple signaling pathways. Understanding the intricate mechanisms of cholesterol motion and its interaction with biological environments is crucial for comprehending its impact on cellular processes. The Niemann-Pick type C1 (NPC1) protein plays a vital role in transporting cholesterol from lysosomes to the endoplasmic reticulum, ensuring its availability for various cellular functions. Likewise, the Niemann-Pick Type C1 Like1 (NPC1L1) protein primarily absorbs cholesterol in the small intestine, contributing to the regulation of whole-body cholesterol levels. Although significant progress has been made in unraveling the mechanisms of these proteins, several questions remain unanswered, hindering our comprehensive understanding of cholesterol homeostasis. Particularly, the initiation signals for the action of NPC1 and NPC1L1, including the role of cholesterol as a potential initiator for other cholesterol homeostasis-related pathways, remain unclear. In this study, we aim to address these knowledge gaps by investigating how the cholesterol content in the membrane surrounding NPC1 and NPC1L1 influences cholesterol trafficking processes within these proteins using molecular dynamics simulations. By employing this approach, we aim to provide valuable insights into the broader picture of cholesterol homeostasis, shedding light on the intricate interplay between cholesterol, membrane environments, and protein dynamics.

P7

Anomalous Dynamical Phase Transitions of the Ising Model Studied by Nonequilibrium Ensemble Method

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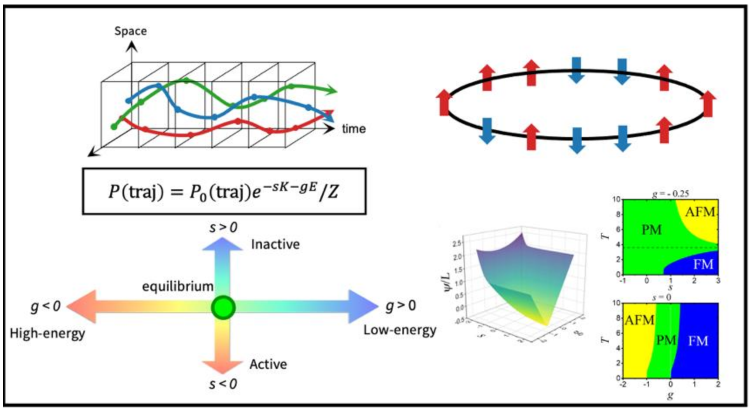
We explore the dynamical phase properties and phase transitions in the one-dimensional Glauber-Ising model using the trajectory ensemble methodology and the large deviation theory. The trajectory ensemble methodology involves a collection of trajectories subject to the same dynamical conditions, resulting in far-from-equilibrium states. While previous studies focused solely on the conjugate variable of dynamical activity, s, our investigation utilizes the double-biased trajectory ensemble method, introducing an additional field g that biases the trajectory energy. By combining these two fields, a decoupling between activity and energy emerges, revealing intriguing phenomena such as freezing by heating and the existence of a permanent liquid state. This study can expand our understanding of non-equilibrium states, offering a new approach to exploring similar phenomena in other systems.



P8

Anomalous Lithium Ion Transport In Ionic Liquids

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Lithium-ion transport is significantly retarded in ionic liquids (ILs). In this work, we performed extensive molecular dynamics (MD) simulations to mimic the kinetics of lithium ions in ILs using [*N*-methyl-*N*-propylpyrrolidium (pyr$_{13}$)][bis(trifluoromethanesulfonyl)imide (Ntf$_2$)] with added LiNtf$_2$ salt. And we analyzed their transport, developing a two-state model and comparing it to the machine learning-identified states. The transport of lithium ions involves local shell exchanges of the Ntf$_2$ in the medium. We calculated train size distributions over various time scales. The train size distribution decays as a power law, representing non-Poissonian bursty shell exchanges. We analyzed the non-Poissonian processes of lithium ions transport as a two-state (soft and hard) model. We analytically calculated the transition probability of the two-state model, which fits well to the lifetime autocorrelation functions of LiNtf$_2$ shells. To identify two states, we introduced the graph neutral network incorporating local molecular structure. The results reveal that the shell-soft state mainly contributes to the transport of the lithium ions, and their contribution is more important in low temperatures. Hence, it is the key for enhanced lithium ion transport to increase the fraction of the shell-soft state.

Intermolecular Interaction-Based Featurization of Small Organic Molecules

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One of the major issues of the machine learning applications on computational chemistry is a limited number of available experimental data, considering the current expansions of the machine learning models in terms of their complexity. For the sake of this issue, in this study, we suggest a strategy that extracts molecular features in the complex, neural network-based model and utilizes them in a simpler, traditional machine learning model that is robust to overfitting. The suggested approach can be applied to predict various properties, such as viscosity or surface tension, of the liquid system from the molecular features drawn from the *ab initio* calculated free energy of solvation. Moreover, we propose a modified kernel model involving the Arrhenius temperature dependence to embed theoretical notions and reduce excessive non-linearity in the model. The modified kernel model demonstrates a significant improvement in specific situations and possible extensions to various theoretical concepts of the molecular system.

P10

Enhanced Sampling for Free Energy Profiles with Post-Transition-State Bifurcations

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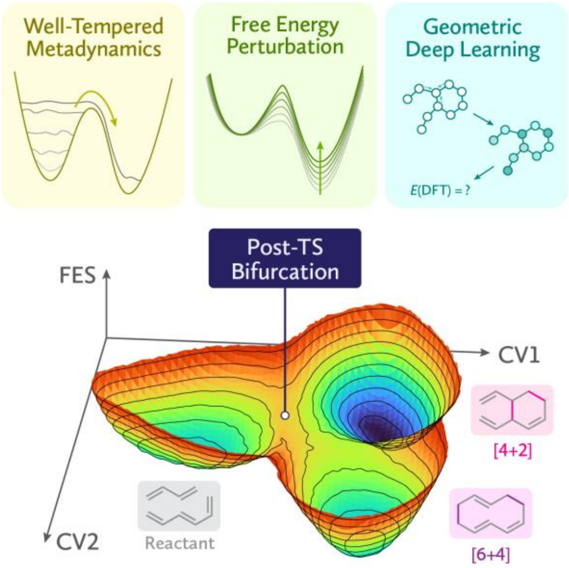
We present a strategy to explore the free energy landscapes of chemical reactions with post-transition-state bifurcations using an enhanced sampling method based on well-tempered metadynamics. Obviating the need for computationally expensive density functional theory-level ab initio molecular dynamics simulations, we obtain accurate energetics by utilizing a free energy perturbation scheme and deep learning estimator for the single-point energies of substrate configurations. Using a pair of easily interpretable collective variables, we present a quantitative free energy surface that is compatible with harmonic transition state theory calculations and in which the bifurcations are clearly visible. We demonstrate our approach with the example of the SpnF-catalyzed Diels–Alder reaction, a cycloaddition reaction in which post-transition-state bifurcation leads to the [4+2] as well as the [6+4] cycloadduct. We obtain the free energy landscapes for different stereochemical reaction pathways and characterize the mechanistic continuum between relevant reaction channels without explicitly searching for the pertinent transition state structures.



P11

Modeling the Charge and Exciton Transports in Organic Semiconductors

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Organic semiconductors (OSs) have been applied to many electronics/optoelectronics such as organic field effect transistors, organic light emitting diodes, biological sensors, and organic solar cells. The attractive features of mechanical flexibility, low manufacturing cost, and abundant availability for the chemical elements render them superior to their inorganic counterparts for novel applications. To further design the devices with improved performance, key material parameters in terms of charge and/or exciton transports must be optimized. However, the detailed mechanisms of these processes are still not fully understood in OSs because of the complexity of the systems. Direct simulations of the nuclear and electronic dynamics for the processes in the material often demand large time and length scales, which are very challenging tasks. Here, we demonstrate nonadiabatic molecular dynamics (NAMD) approaches based on fragment orbital basis to efficiently consider the charge and/or exciton transports in OSs. We show that by combining charge-transfer (CT) and excitonic (XT) blocks of Hamiltonian and adding the CT-XT couplings, the method can describe the exciton dissociation processes in organic donor-acceptor interfaces. Furthermore, we propose to utilize machine-learning methods to accelerate and accurately compute the diabatic couplings (off-diagonal Hamiltonian elements) in every NAMD step, thus an improved description of the electronic Hamiltonian can be expected.

Theoretical Studies on Ultrafast Intramolecular Triplet-Triplet Annihilation

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Triplet-triplet annihilation photon upconversion (TTA-UC) is a process that allows two low-energy photons to combine into one high-energy photon. This process has many applications, such as organic light emitting diodes (OLEDs), solar cells, bioimaging, and more. The efficiency of TTA-UC depends on the diffusion and interaction of triplet excitons between molecules. Intramolecular triplet–triplet annihilation (intra-TTA) has been developed to overcome the inefficiency of molecular diffusion and has been applied in solid-state systems.[1,2]. Olesund et al. proposed two models of intramolecular TTA (intra-TTA), which are double-sensitization (DS) and triplet energy transfer between annihilators (TETA) models and performed time-resolved simulations. We observed that the rate constant of intra-TTA was empirical in the simulation[3]. With the advantage of *ab initio* method, we can calculate the rate constant of intra-TTA using Fermi's golden rule. We used the restricted-active-space configuration-interaction (RASCI) and fragment excitation difference (FED) methods to calculate the electronic coupling of triplet–triplet annihilation (TTA). The ultrafast intra-TTA rate constants for anthracene dimers obtained were in the range of 10^{15} to $3\text{x}10^{12}$ s^{-1}, which are faster than the previously reported value of 10^{15} s^{-1}. The result of time-resolved simulation remained the same as in previous work when using values from ab initio methods.

After extensive experiments and analysis, we came to the conclusion that intra-TTA is not the rate-limiting step in the kinetics of TTA reaction. Instead, we found evidence that intermolecular triplet energy transfer (inter-TET) may have a significant influence on the outcome.

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GWANAK CAMPUS MAP

HOW TO USE

SNU Gwanak campus has more than 200 buildings, all of which have their own numbers. The map is divided into 11 zones, using area codes A–K.

Note that some buildings are not listed below.

BUILDINGS

H	1~8, 14	College of Humanities
H	4	Shinyang Humanities Hall
H	9~13	College of Education
B	15, 15-1, 17	School of Law
B	16	College of Social Sciences
B	16-1	Shinyang Social Sciences Hall
G C	18~19, 22~28	College of Natural Sciences
C G	20~21 29	College of Pharmacy
E	30~43-1	College of Engineering
G	44-1	Shinyang Engineering Hall
G F	45~46, 48, 48-1 47	Observatories
I	49	Design Center & Concert Hall
I	50~52	College of Fine Arts
I	53~55	College of Music
C	56	College of Natural Sciences
I	57, 57-1	Graduate School of Public Administration
I	58	College of Business Administration
I	59	Graduate School of Business
C	60	**Administration Building**
H	61	Center for Teaching and Learning
C	62, 62-1	**University Library**
C	63	Student Center
B	64	IBK Communication Center
G	65	Faculty Club
B	67	Dure Cultural Center
G	69	● Institute of Laboratory Animal Resources
I	70	University Museum
A	71	Gymnasium
A	71-1	Sports Education and Research Building
A	71-2	POSCO Sports Complex
B	72	Law Library
C	73	University Cultural Center
I	74	Arts Education & Research Building
D	75	University Newspaper
D H	75-1 76	Cafeteria
A	80	Veterinary Medical Teaching Hospital
I	82	Graduate School of Environmental Studies
B	83	Multimedia Lecture Building II
B	84	Centennial Building, College of Law
A	85	College of Veterinary Medicine
A	86	SNU Dental Hospital in Gwanak
A	97~98	Institute of Environmental Protection and Safety
G	100	Poongsan Outdoor Theater
B	101	Asia Center
C	102	Office of Information Systems and Technology
C	103	Kyujanggak Archives
G	104	Inter-University Semiconductor Research Center
G	105	Institute for Molecular Biology & Design
H	109	Cafeteria Jahayon
H	111	Café
I	113	Dongwon Dining Hall
K	122	Faculty Apartments A-I
K	125~127	Hoam Faculty House
C	129	Sangsan Mathematical Sciences Building
E G	130~131, 133 132, 135 138~139	College of Engineering
A	137, 137-1	**Language Education Institute**
A	137-2	Daelim International House
I	140~140-2	Graduate School of International Studies
G	141~143	College of Pharmacy
A	150	**Office of Admissions**
A	151	Museum of Art (MoA)
A	152	**Office of International Affairs**
A	152-1	Lotte International Hall
A	153	Woojeongwon
D	200	College of Agriculture and Life Sciences
I	220	College of Liberal Studies
I	221	Graduate School of Public Health
I	222	College of Human Ecology
F	300	● RYU Hoi Jin Library
F	301~302	College of Engineering
F	310	Engineer House
F	311~316	College of Engineering
D	500	College of Natural Sciences
J K	900~906, 918~926 931~935	Student Residence
K	907~909	● Global Student Residence
K	936	Staff Apartments
K	940	Research Park Building
K	941	Child Educare Center
K	942~945	R&DB Centers
K	946	**BK International House**
K	950	International Vaccine Institute

● Under Construction

Chemistry Dept.

Hoam Faculty House

Office of International Affairs (OIA) bldg. 152

1 Gwanak-ro, Gwanak-gu, Seoul 08826

G Gate to parking area
P Open parking area
🟩 Bus stops
Airport Limousine
— Roadway
✚ Health care
Dining
Cafés

Map of Hoam Faculty House