# PROGRAM AND ABSTRACTS

## TMCQ 2024

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

July 8-12, 2024

Seoul, Korea

**ORGANIZED BY**

Cheol Ho Choi (Kyungpook National University)

Changbong Hyeon (KIAS)

Seogjoo J. Jang (CUNY-Queens College)

YounJoon Jung (Seoul National University)

Chang Woo Myung (Sungkyunkwan University)

**HOST**

School of Computational Sciences, KIAS

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# Welcoming Remarks

It is our great pleasure to welcome all of you to the second International Workshop on New Advances in Theoretical and Computational Molecular Sciences for Complex and Quantu Processes (TMCQ2024) at Korea Institute for Advanced Study (KIAS).

The workshop will provide great opportunities for leading scholars to discuss recent advances and challenging issues in theoretical and computational molecular sciences. During five days of workshop at KIAS, participants will enjoy close interactions and open discussions in a friendly environment. We hope this workshop offers you a unique opportunity to conceive new ideas on the basis of firm foundations of theories and computational methods developed for decades.

Organizing Committee,

Cheol Ho Choi (Kyungpook National University)

Changbong Hyeon (KIAS)

Seogjoo Jang (CUNY-Queens College)

YounJoon Jung (Seoul National University)

Chang Woo Myung (Sungkyunkwan University)

# Introduction to TMCQ2024

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

| July 8 (Mon) | | July 9 (Tue) | | July 10 (Wed) | | July 11 (Thu) | | July12 (Fri) |
|---|---|---|---|---|---|---|---|---|
| 8:30 -10:00 | Breakfast/ Registration | 8:30 -9:30 | Breakfast | 8:30 -9:30 | Breakfast | 8:30 -9:30 | Breakfast | Free Discussion |
| | Opening Remark | | | | | | | |
| **Session 1: S. J. Jang** | | **Session 3: Y.W. Son** | | **Session 5: J. Schultz** | | **Session 7: C. W. Myung** | | |
| 10:00 -10:40 | A. Nitzan | 9:30 -10:10 | G. Schatz | 9:30 -10:10 | N. Makri | 9:30 -10:10 | A. Tkatchenko | |
| 10:40 -11:00 | H. Kim | 10:10 -10:50 | J. Jang | 10:10 -10:50 | Y. H. Jang | 10:10 -10:30 | C. H. Choi | |
| 11:00 -11:20 | Break | 10:50 -11:10 | Break | 10:50 -11:10 | Break | 10:30 -10:50 | Break | |
| 11:20 -12:00 | Y.W. Son | 11:10 -11:50 | G. Chan | 11:10 -11:50 | Y. W. Kim | 10:50 -11:30 | Y. Jung | |
| | | | | | | 11:30 –11:50 | S. Jang | |
| 12:00 -14:00 | Lunch | 11:50 -12:10 | J. D. Schultz | 11:50 -12:10 | J. H. Kim | 12:00 -13:10 | Lunch | |
| | | 12:10 -14:00 | Lunch | 12:10 -14:00 | Lunch | | | |
| **Session 2: Y. Jung** | | **Session 4: C. H. Choi** | | **Session 6: C. Hyeon** | | | | |
| 14:00 -14:40 | P. Rossky | 14:00 -14:40 | J. Liu | 14:00 -14:40 | Y. Tanimura | | | |
| 14:40 -15:00 | J. M. Choi | 14:40 -15:00 | S. Lee | 14:40 -15:00 | H. W. Cho | | | |
| 15:00 -15:20 | Break | 15:00 -15:20 | Break | 15:00 -15:20 | Break | 13:10 | Excursion & Free Hour | |
| 15:20 -16:00 | H. Hwang | 15:20 -16:00 | W. Y. Kim | 15:20 -16:00 | A. Izmaylov | | | |
| 16:00 -16:40 | J.E. Shea | 16:00 -18:00 | Poster Session with drink & refreshments | 16:00 -16:20 | J. Huh | | | |
| | | | | 16:20 -17:00 | Transportation to banquet | | | |
| | | | | 17:00 -18:30 | Banquet (for all participants) | | | |

# PROGRAM

| July 8 (Mon) | | |
|---|---|---|
| 8:30-10:00 | | Breakfast/Registration |
| | | Opening Remark |
| | **Session 1: Seogjoo J. Jang (CUNY-Queens)** | |
| 10:00-10:40 | Abraham Nitzan (Univ. of Pennsylvania) | Collective response in light-matter Interactions: The interplay between strong coupling, local dynamics, and disorder |
| 10:40-11:00 | Hyungjun Kim (Incheon National Univ.) | Diverse Quantum Interference Regime in Intramolecular Singlet Fission |
| 11:00-11:20 | | Coffee Break |
| 11:20-12:00 | Young-Woo Son (KIAS) | Ab initio extended Hubbard interactions and their applications |
| 12:00-14:00 | | Lunch |
| | **Session 2: Younjoon Jung (Seoul Nat'l Univ.)** | |
| 14:00-14:40 | Peter Rossky (Rice Univ.) | Identifying "molecular scenarios" that underlie experimental observations |
| 14:40-15:00 | Jeong-Mo Choi (Pusan National Univ.) | Network Structure and Dynamics of Biomolecular Condensates |
| 15:00-15:20 | | Coffee Break |
| 15:20-16:00 | Hyonseok Hwang (Kangwon National Univ.) | Exploring Surfactant Micelles and Cancer Drugs Interacting with Cell Membranes |
| 16:00-16:40 | Joan-Emma Shea (UC Santa Barbara) | Self-assembly of the Tau protein: Liquid-liquid phase separation and fibrillization |
| 17:30 | | Reception with Invited Speakers |

| July 9 (Tue) | | |
|---|---|---|
| 8:30-9:30 | | Breakfast |
| | **Session 3: Young-Woo Son (KIAS)** | |
| 9:30-10:10 | George Schatz (Northwestern Univ.) | Plasmons, molecules and theory: where Top-down meets Bottom-up |

| | | |
|---|---|---|
| 10:10-10:50 | Joonkyung Jang (Pusan National Univ.) | Molecular Structure and Phase Transition of Interfacial Water |
| 10:50-11:10 | | Coffee Break |
| 11:10-11:50 | Garnet Chan (Caltech) | Two or more short stories |
| 11:50-12:10 | Jonathan D. Schultz (Duke Univ.) | Leveraging machine learning to disentangle electronic couplings from congested two-dimensional electronic spectra |
| 12:10-14:00 | | Lunch |
| | **Session 4: Cheol Ho Choi (Kyungpook Nat'l Univ.)** | |
| 14:00-14:40 | Jian Liu (Peking Univ.) | Nonadiabatic Field: A Conceptually Novel Approach for Nonadiabatic Dynamics |
| 14:40-15:00 | Seunghoon Lee (Seoul National Univ.) | Computing X-ray spectra of transition-metal clusters based on matrix product states |
| 15:00-15:20 | | Coffee Break |
| 15:20-16:00 | Woo Youn Kim (KAIST) | Automate transition state calculations with chemical heuristics and AI |
| 16:00-18:00 | | Poster Session with drink & refreshments |

| **July 10 (Wed)** | | |
|---|---|---|
| 8:30-9:30 | | Breakfast |
| | **Session 5: Jonathan D. Schultz (Duke Univ.)** | |
| 9:30-10:10 | Nancy Makri (Univ. of Illinois, Urbana-Champaign) | Real-time path integral methods for quantum dynamics |
| 10:10-10:50 | Yun Hee Jang (DGIST) | Hard-Cation-Soft-Anion Ionic Liquids for PEDOT:PSS Conductivity Enhancement. Multiscale Molecular Modeling |
| 10:50-11:10 | | Coffee Break |
| 11:10-11:50 | Yong Woon Kim (KAIST) | Target searches by active particles |
| 11:50-12:10 | Ji-Hyun Kim (Chung-Ang Univ.) | Integrated method for identifying the optimal descriptor of acute critical illness: Development of septic infection related risk index (SIRRI) and investigation into patient's fate dynamics along SIRRI |
| 12:10-14:00 | | Lunch |

**Session 6: Changbong Hyeon (KIAS)**

| | | |
|---|---|---|
| 14:00-14:40 | Yoshitaka Tanimura (Kyoto Univ.) | Classical and quantum thermodynamics in non-equilibrium regime: The dimensionless minimum work principle |
| 14:40-15:00 | Hyun Woo Cho (Seoultech) | Universal Transport Distribution in Percolation |
| 15:00-15:20 | | Coffee Break |
| 15:20-16:00 | Artur Izmaylov (Univ. of Toronto) | Algebraic techniques for quantum computing in quantum chemistry |
| 16:00-16:20 | Joonsuk Huh (Sungkyunkwan Univ.) | Perfect Matching with Photons, Phonons, Electrons, and Spins |
| 16:20-17:00 | | Transportation to banquet |

**July 11 (Thu)**

| | | |
|---|---|---|
| 8:30-9:30 | | Breakfast |

**Session 7: Chang Woo Myung (Sungkyunkwan Univ.)**

| | | |
|---|---|---|
| 9:30-10:10 | Alexandre Tkatchenko (Univ. of Luxembourg) | Towards quantum force fields using quantum charged oscillators |
| 10:10-10:30 | Cheol-Ho Choi (Kyungpook National Univ.) | MRSF-TDDFT: A Breakthrough for DFT/TDDFT |
| 10:30-10:50 | | Coffee Break |
| 10:50-11:30 | Yousung Jung (Seoul National Univ.) | Organic Synthesis Predictions Enabled by AI |
| 11:30–11:50 | Seogjoo Jang (CUNY-Queens College) | Magnus Expansion for Quantum Dynamical Processes |
| 12:00-13:10 | | Lunch |
| 13:10 ~ | | Excursion |

**July 12 (Fri)**

| |
|---|
| Free Discussion |

# ABSTRACTS OF TALKS

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Session 2

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Session 5

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Session 7

Session 8

Session 9

Session 10

# Collective response in light-matter interactions: The interplay between strong coupling, local dynamics, and disorder

**A. Nitzan**

*University of Pennsylvania and Tel Aviv University*

Because molecular size is much smaller than optical wavelength molecules can interact with light collectively. Actual manifestations of such collective response depend on other factors such as dephasing and disorder. Under strong (molecules-light) coupling conditions such collective response can be more pronounced because collective modes are energy-shifted from the spectrum of individual emitters and appear as polaritonic spectral features in linear and non-linear optical signals. In this talk, I will describe our recent studies of several phenomena that reflect this interplay between collective response, local dynamics, and (static and dynamic) disorder.

# Diverse Quantum Interference Regime in Intramolecular Singlet Fission

**Jonghwan Lee, Sungsik Eom, and Hyungjun Kim**

*Department of Chemistry, Incheon National University, Incheon 22012, South Korea*

An array of thiophene-based π-conjugated linkers in covalently-linked pentacene dimers allows us to access diverse quantum interference (QI), modulating nonadiabatic coupling (NAC) in singlet fission (SF) process. Simulations show that structural isomerism in terms of S atom orientation substantially alters NAC with relatively marginal impacts on energies. Extended curly arrow rules (ECARs) reveal sensitive dependence of QI on SF linker topologies and connectivity, categorizing regimes of constructive, destructive, and previously unrealized in SF research, suppressed destructive QI. Drastic NAC changes in terms of S atom orientation are rationalized based on the nature of QI. Our results from nonequilibrium Green's function calculation using density functional theory corroborates the classification of QI regimes based on ECARs. Moreover, we found that the extent of charge resonance contribution in electronic states relevant to multiexciton formation and the appearance of optically allowed charge transfer excitation strongly depends on the operative QI regime. Notably, the magnitude of NAC effectively captures this influence. Our findings show that QI can rationalize and semi-quantitatively correlate to NAC for multiexciton formation step in SF process.

# Ab initio extended Hubbard interactions and their applications

**Young-Woo Son**

*School of Computational Sciences, Korea Institute for Advanced Study, Seoul, South Korea*

For massive database-driven materials research, there are increasing demands for both fast and accurate quantum mechanical computational tools. Contemporary methods can be fast, sacrificing their accuracy, or be precise, consuming a significant amount of resources. In this talk, to overcome such a problem, I will present my group's recent efforts on systematic improvements of self-interactions error corrections in first-principles calculations based on density functional theory (DFT). I will present theories and implementations [1-3] on efficient ways of computing position-dependent self-consistent on-site and inter-site Hubbard interactions and their fully relativistic extension. Owing to a low computational cost of the new method comparable to DFT and improved accuracy to the *GW* approximation, the new method provides an opportunity to study the correlated solids in large scale structures and full phase space of interests. A few examples of applications such as charge order systems, metal oxides, few layer graphene and ferroelectric perovskite oxides [4-7] will be demonstrated to show superior performance and accuracy of our new method.

[1] S.-H. Lee and Y.-W. Son, Phys. Rev. Res. **2**, 043410 (2020).
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[3] W. Yang and Y.-W. Son, *in preparation* (2024).
[4] W. Yang *et al*., J. Phys. Condens. Metter **34**, 295601 (2022).
[5] B. G. Jang *et al*., Phys. Rev. Lett. **130**, 136401 (2023).
[6] D. Lee *et al*., arXiv:2403.00530 (2024).
[7] M. C. Choi *et al.*, *in preparation* (2024).

# *Identifying "molecular scenarios" that underlie experimental observations*

**Peter J. Rossky**

*NSF Center for Adopting Flaws into Features*
*Department of Chemistry and Department of Chemical & Biomolecular Engineering*
*Rice University*

Theoretical methods and algorithms have made great strides in their capacity to faithfully describe complex molecular systems, while, in parallel, there has been an enormous increase in the capability of and access to high performance computing resources. As a result, there is now a realistic expectation that theory and experiment should function in a symbiotic relationship to resolve the molecular mechanisms underlying interesting laboratory phenomena, and, ideally, point to experimental refinements, e.g., of the molecular composition of a material. A key challenge is that the molecular *structures* present are often not *a priori* known. Hence, one first must postulate one or more "molecular scenarios", including structure and potential mechanism, and then use calculations to determine whether such a scenario leads to observables *consistent* with experiment. In this talk, I will discuss examples of this process for observed photoexcited state dynamics. The examples will include results from study of semiconducting conjugated polymers and from studies of excited state "singlet fission" in a molecular crystal.

# Network Structure and Dynamics of Biomolecular Condensates

**Jeong-Mo Choi[1]**

*[1]Department of Chemistry, Pusan National University, Busan 46241, Republic of Korea*
**E-mail: jmchoi@pusan.ac.kr*

There is growing interest in uncovering the fundamental principles of liquid-liquid phase separation (LLPS) of multivalent proteins with intrinsically disordered regions, given the direct relevance to the reversible formation/dissolution of biomolecular condensates. However, despite recent advances in the field, achieving multiscale structural characterization of these liquid condensates remains an outstanding challenge. Nucleophosmin (NPM1) stands out as a key component of the liquid-like granular component (GC) within the nucleolus. To gain insight into these systems, a minimal model of NPM1, designated as N130, has been developed. This minimal model, N130, encompasses the N-terminal fragment of NPM1, retaining two acidic tracts and the ability to oligomerize into homopentamers. Notably, N130 has the capacity to induce LLPS in the presence of arginine-rich (R-rich) peptides.

In this presentation, I will discuss our recent investigation on phase separation involving various combinations of N130 and R-rich peptides. Our study aimed to decipher the structural nuances of the resulting phase-separated condensates, employing small-angle neutron scattering (SANS) measurements. Additionally, we employed theoretical models and multiscale computer simulations to unveil the intricate molecular characteristics underlying the experimental structural profiles. Collectively, these experimental and theoretical insights not only contribute to our current understanding but also pave the way for a quantitative comprehension of the liquid-like attributes within the NPM1-rich GC region of the nucleolus in the future.

# Exploring Surfactant Micelles and Cancer Drugs Interacting with Cell Membranes

**Hyonseok Hwang**

*Department of chemistry and Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon-si Gangwon-do, Republic of Korea*

Surfactant micelles and drug molecules interacting with cell membranes play a crucial role in drug delivery systems. In this talk, we present a molecular dynamics (MD) simulation study on the behavior of a surfactant micelle and a canter drug on cell membranes. In the first part of the talk, we investigate the charactersistic behavior of sodium lauryl 2-ether sulfate (SLE2S), an anionic surfactant, on model DMPC and ceramide lipid bilayers. Two-dimensional potential of mean force (2D-PMF) calculations reveal that the shape of a single SLE2S micelle depends on the polarity of lipid head groups in the bilayers. surfactant transfers from the SLE2S micelle to the ceramide bilayer were also observed. PMF profiles for the surfactant transfer at different temperatures demonstrate that the energy barriers for the transfer are substantially reduced in the ceramide bilayer as the temperature increases. In contrast, the temperature dependence of the energy barrier was negligible for the DMPC bilayer, and no transfer of surfactants was observed regardless of temperature variation. In the second part of the talk, we address the impact of protonation state and membrane lipid composition on the membrane permeation of doxorubicin (DOX). The free energy profiles revealed that a higher concentration of CHOL in the lipid bilayer leads to a larger energy barrier regardless of protonation state of DOX, but a more rapid increase in the energy barrier was observed in the case of protonated DOX. We also discovered that DOX exhibits different permeation mechanisms depending on protonation state: “solubility diffusion” for neutral DOX and “ion-induced defect” for protonated DOX. The calculated effective permeability coefficients of model systems indicate a strong inhibitory effect of membrane CHOL on DOX permeation, which is further enhanced by drug protonation.

# Plasmons, molecules and theory: where Top-down meets Bottom-up

**George C. Schatz**

*Northwestern University, Evanston IL 60208*

Plasmons are collective excitations of electrons, in which the excited state involves a superposition (entanglement) of electron/hole excitations. This is in contrast with the low lying excited states of most molecules where the excitations correspond to transfer of an electron from an occupied to an unoccupied orbital. Plasmon excited states exist in all molecules and solids but they are most commonly studied in silver and gold nanoparticles, there they are responsible for the vivid colors of colloidal silver and gold. It is possible to describe the optical properties of plasmonic materials using classical electrodynamics with an empirical dielectric function, and this is extremely useful for applications in nanoscience, as it enables the description of metal structures that are hundreds of nm in size. However properties that involve the transfer of charge between the metal and adsorbed molecules cannot be described this way, and it is necessary to use quantum chemistry methods instead. This sort of calculation was originally done in the 1980s, but it is only in the last 20 years that the calculations have become meaningful, as there are now metal cluster materials with well-defined structures which have been studied experimentally. In addition, calculations on metal clusters that are a few nm in size provide a very good model for the properties of 10-100nm size particles when describing such phenomena as the chemical effect in SERS, the effects of pressure on optical spectra, or plasmon-induced photocatalysis. Although many of the calculations can be done using standard electronic structure codes, there is also an important role for new theory development. To describe plasmonic photocatalysis, an important new development has been the emergence of tight-binding semiempirical methods, which enable the description of plasmonic clusters with 1000 atoms and more, and including for real-time TDDFT calculations. Here we report on new directions in plasmonics that have been enabled by these methods.

# Molecular Structure and Phase Transition of Interfacial Water

**Seyong Choi, Kiduk Kim, Jaeyoung Kim, and Joonkyung Jang***

*Department of Nano-energy Engineering, Pusan National University, Busan 46241, Republic of Korea*

Many chemical and biological processes involve interfacial water much different from the bulk in structure and phase behavior. Using molecular simulation and theory, we examine the molecular structure and phase behavior of an interfacial water. Atomic force microscopy (AFM) and vibrational-sum-frequency-generation spectroscopy are used to probe the molecular structure of an interfacial water. We show a molecular simulation is helpful for a clear interpretation of these experiments. We investigate the drying transition of the interfacial water as an AFM tip approaches a hydrophobic surface. Implications of these results for interpreting an AFM measurement are discussed. Controlling the wettability of a surface with an array of the micro(nano)scale pillars finds wide applications. We study the wetting transition of the interfacial water contacting a nano-corrugated surface. We uncover the metastable and transition states in the wetting transition. The wettability of a pillared surface is quantified by the contact angle (CA) of a water droplet. It is desired to know the CA prior to construction of pillars, in order to obviate the trial-and-errors of experimenting with different topographies. Given the difficulty of theoretical prediction of CA, we propose a convolutional neural network (CNN) model of CA. By employing a three-dimensional descriptor of the surface topography, our CNN model can predict experimental CAs within errors comparable to the experimental uncertainties in measuring CAs.

# Two or more short stories

**Garnet Chan**

*California Institute of Technology, Pasadena, CA, USA.*

In the first part of my talk, I will describe recent advances in the ab initio simulation of correlated quantum materials, in particular, the high temperature superconductors. In the second part of my talk, I will describe our efforts towards understanding the reaction mechanism of nitrogenase by bridging timescales. If time permits, I will briefly mention some conceptual work in quantum dynamics in the area of influence functionals.

# Leveraging machine learning to disentangle electronic couplings from congested two-dimensional electronic spectra

**Jonathan D. Schultza, Kelsey A. Parkera, Bashir Sbaitia, and David N. Beratana,b,c***

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*b Department of Physics, Duke University, Durham, NC, 27708, USA*
*c Department of Biochemistry, Duke University, Durham, NC, 27710, USA*

Two-dimensional electronic spectroscopy (2DES) is mobilizing physical chemistry research by affording rich insight into the mechanisms of light-driven processes. Theoretically, 2DES data provide a detailed roadmap of a molecular sample's vibronic degrees of freedom. In practice, however, much of the chemical insight contained in 2DES spectra is masked by overlapping spectral features, sample heterogeneities, and background noise. Accurate and comprehensive methods to disentangle key molecular properties from 2DES datasets will be indispensable as this technique is used to study increasingly complex molecular systems. Here, we explore the capacity of neural networks to extract electronic couplings from 2DES spectra of condensed-phase systems. We leverage a targeted training database of numerically simulated spectra that encode vibronic exciton dynamics across a wide range of Hamiltonian parameters. We show that neural networks can translate previously unseen spectra into highly accurate predictions of the underlying electronic couplings. Furthermore, we highlight efforts to bridge simulation-trained neural networks toward experimental contexts and discuss the prospects for machine learning to transform how chemical insight is gleaned from 2DES experiments.

# Nonadiabatic Field

***Jian Liu*** [1]

[1] *Beijing National Laboratory for Molecular Sciences, Institute of Theoretical and Computational Chemistry, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China*

Nonadiabatic transition dynamics lies at the core of many electron/hole transfer, photoactivated, and vacuum field-coupled processes. About a century after Ehrenfest proposed "Phasenraum" and the Ehrenfest theorem, we report a conceptually novel trajectory-based nonadiabatic dynamics approach, nonadiabatic field (NaF), based on a generalized exact coordinate–momentum phase space formulation of quantum mechanics, which includes U(F)/U(F-1) constraint phase space for electronic degrees of freedom (DOFs) and infinite phase space for nuclear DOFs. It does not employ the conventional Born–Oppenheimer or Ehrenfest trajectory in the nonadiabatic coupling region. Instead, in NaF the equations of motion of the independent trajectory involve a nonadiabatic nuclear force term in addition to an adiabatic nuclear force term of a single electronic state. A few benchmark tests for gas phase and condensed phase systems indicate that NaF offers a practical tool to capture the correct correlation of electronic and nuclear dynamics for processes where the states remain coupled all the time as well as for the asymptotic region where the coupling of electronic states vanishes.

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[3] X. He, J. Liu, *J. Chem. Phys.* **151**, 024105 (2019)
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[8] B. Wu, X. He, J. Liu, *J. Phys. Chem. Lett.* **15(2)**, 644-658 (2024)
[9] X. Cheng, X. He, J. Liu, *Chin. J. Chem. Phys.* **37(2)**, 230-254 (2024)
[10] X. He, X. Cheng, B. Wu, J. Liu, *J. Phys. Chem. Lett.* **15(20)**, 5452–5466 (2024)

# Computing X-ray spectra of transition-metal clusters based on matrix product states

**Seunghoon Lee**

*Department of Chemistry, Seoul National University, Seoul 08826, Republic of Korea*

We are developing a new theoretical approach for computing spectra of the L-edge X-ray absorption spectroscopy (XAS) and the 2p3d resonant inelastic X-ray scattering (RIXS) spectroscopies. [1] This novel approach allows to compute the spectra without the need for excited-state wave functions and energies, thereby significantly reducing computational overhead. Moreover, the utilization of matrix product states and sweep algorithms further reduces the cost. This approach is particularly advantageous for strongly correlated systems, such as iron-sulfur complexes, which have a large number of intermediate and final states.

Iron-sulfur complexes carry out a wide range of biological functions including electron carrier, sensor, and catalyst. Understanding detailed electronic properties and electronic structure of these complexes is of importance, yet still remains a challenging task. Along with experimental advances, the L-edge XAS and the 2p3d RIXS spectroscopies provide high-intensity and high-resolution spectra rich in information of the electronic structure. However, the interpretation of the L-edge XAS and 2p3d RIXS spectra is extremely challenging.

Recently, various ab-initio methods have been used to simulate and to interpret the spectra, including restricted open-shell configuration interaction (ROCIS) [2], restricted active space self-consistent field (RASSCF) [3], and multi reference CI (MRCI) [4]. However, all the methods require the explicit wavefunctions of the intermediates and the final states. Although these approaches have been successful in many small-size molecular systems, these have clear limitations to compute the spectra of the metal clusters. The new method we propose can address the shortcomings and show a good agreement between the experimental and theoretical spectra using active space models that employ the ab-initio Hamiltonian with spin-orbit coupling. In addition, we compute the XAS and RIXS spectra of the iron-sulfur dimer in the first time. We believe that the new method opens a new possibility to unveil the electronic structure of the iron-sulfur clusters through comparisons with experimental spectra.

**References**

[1] S. Lee, H. Zhai, and G. K. Chan, *J. Chem. Theory Comput.*, **19**, 7753 (2023)

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# Automate transition state calculations with chemical heuristics and AI

**Woo Youn Kim**[1]

[1] *Department of Chemistry, KAIST, Daejeon, Korea*

Despite remarkable advances in computational chemistry, automated transition state calculations are still challenging due to high structural complexities around transition states. It first needs to find appropriate molecular orientations between reactant molecules, which are typically done manually. Given the predetermined orientation, one can search a transition state by exploring a potential energy surface starting from the reactant state all the way to the respective product state, for example, with single-ended or double ended methods. Here, we present a fully automated approach to searching transition states of a given chemical reaction. To avoid huge computational bottleneck for automation, we utilize chemical heuristics in searching appropriate molecular orientations of reactant and product molecules and in approximating transition states from the orientation information. Our benchmark study shows that the proposed method can find transition states of typical organic reactions very accurately in a fully automated fashion. To further accelerate the process, we introduce deep learning techniques. They can replace chemical heuristics and expensive calculations with a data-driven approach. Specifically, we adopted a diffusion-based generative AI for searching transition states directly from graph information of reactants and products.

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# Real-Time Path Integral Methods for Quantum Dynamics

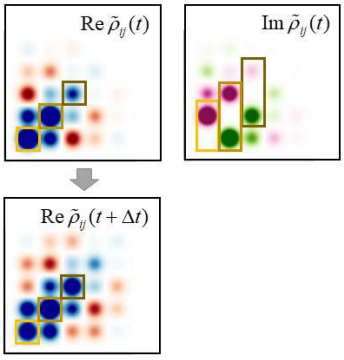
**Nancy Makri**

*University of Illinois at Urbana-Champaign*

The unfavorable scaling of wavefunction storage severely impacts the feasibility of quantum dynamical calculations on large molecular and condensed-phase systems. Feynman's path integral formulation offers an attractive alternative, replacing wavefunctions by a sum of quantum mechanical amplitudes along all possible paths. However, the path sum involves astronomical numbers of terms, and stochastic methods are unable to deal with the oscillatory quantum phase.

A series of developments have led to rigorous and efficient real-time path integral methods that allow the accurate simulation of exciton-vibration dynamics. The *quasi-adiabatic propagator path integral* (QuAPI) for system-bath dynamics achieves linear scaling with the number of time steps by propagating a tensor that spans the memory interval. Recent work showed that one can further disentangle the path integral variables through the *small matrix decomposition* (SMatPI), which eliminates tensor storage, enabling the simulation of long-memory processes and multistate systems. The SMatPI propagation matrices are obtained by evaluating full- or extended-memory path sums, which are accelerated through blip, kink, or other decompositions. The *modular path integral* (MPI) algorithm for extended systems (composed of many units, each with its own vibrational /phonon bath, interacting locally) offers linear scaling with the aggregate length. These methods converge to exact, fully quantum mechanical results with any number of harmonic modes, at zero or finite temperature. The *quantum-classical path integral* (QCPI) offers a rigorous formulation of nonadiabatic dynamics in solution or biological environments. These path integral methods capture the complex interplay among quantum coherence, delocalization, vibrational damping and thermal fluctuations in dynamical processes.

Further, it is shown that the reduced density matrix (RDM) contains all the necessary information to infer the instantaneous state-to-state rates (SSR) that govern the dynamics. *Coherence maps* offer a powerful visualization tool for understanding the creation and destruction of quantum superpositions and enable a state-to-state pathway analysis of dynamical processes.

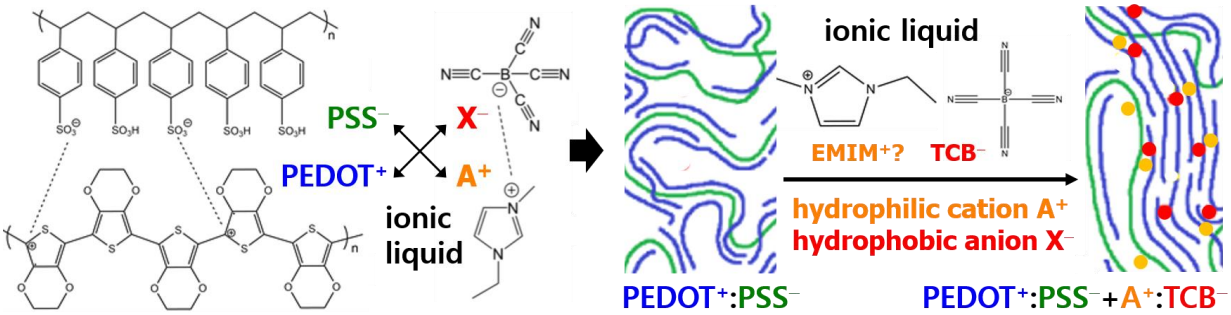


# Hard-Cation-Soft-Anion Ionic Liquids for PEDOT:PSS Conductivity Enhancement. Multiscale Molecular Modeling

**Changwon Choi,[1] Ambroise de Izarra,[1,2] Yves Lansac,[2,3] Yun Hee Jang[1]**

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Water-processable mixtures of positively-charged poly-3,4-ethylenedioxythiophene (PEDOT) and negatively-charged polystyrenesulfonate (PSS) have received great attention as a flexible, stretchable, conformable, lightweight, transparent, and low-cost organic (semi)conductor and electrochemical transistor, which can be used for applications such as organic LED, solar cell, thermoelectric genera-tor, self-powered implantable sensor and actuator, and artificial skin. They form 10-to-30-nm granular domains, where conducting-but-hydrophobic PEDOT-rich regions are surrounded by hydrophilic-but-insulating PSS-rich regions, hindering formation of large conducting PEDOT domains. It makes PEDOT:PSS water-soluble, thermally stable, and environmentally benign, but poor in conductivity. Adding polar organic solvents, acids, or organic/inorganic salts to the PEDOT:PSS solution has enhanced the conductivity by 2-3 orders of magnitude. Recently, remarkable 5,000-fold improvement of conductivity has been achieved by mixing proper ionic liquids (ILs) in a PEDOT:PSS solution of deionized water and polar organic solvents.[1-2] In a series of free energy calculations using density functional theory and molecular dynamics simulations[2-6] based on the classic "hard soft acid (cation) base (anion)" principle, we have demonstrated the followings: (1) ion exchange between $PEDOT^+$:$PSS^-$ and $A^+$:$X^-$ ILs would help $PEDOT^+$ to decouple from $PSS^-$ and to grow into large-scale conducting domains of π-stacked $PEDOT^+$ decorated by IL anions $X^-$; (2) the most spontaneous decoupling between *hydrophobic/soft* $PEDOT^+$ and *hydrophilic/hard* $PSS^-$ would be induced by strong interaction with *hydrophobic/soft* anions $X^-$ and *hydrophilic/hard* cations $A^+$, respectively; and (3) the most efficient IL anions $X^-$ remaining in the PEDOT domain after the ion exchange would sustain the highest amount of charge carriers uniformly distributed along the PEDOT backbone to further enhance the conductivity as well as stretchability.[7]



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# Target searches by active particles

**Yong Woon Kim**

*KAIST*

How long will it take for a blind searcher to find a target in a confined space? This is a central question in the random target search or the first-passage process, which plays a pivotal role in understanding a variety of phenomena ranging from diffusion-limited reactions, predator foragings to intracellular protein transports. We discuss random target search of a partially absorbing target by an active particle. We find that the mean searching time shows a non-monotonic behavior as a function of the self-propulsion speed of the active particle, indicating the existence of an optimal speed, when the absorption strength of the target is finite. As a practical application exploiting the existence of the optimal speed, we propose a filtering device to extract active particles with a desired speed and evaluate how the resolution of the filtering device depends on the absorption strength. As thermal noise of environment increases, the optimal velocity changes from a finite value to zero, which implies that a purely diffusive Brownian motion outperforms an active motion in terms of searching time. Depending on the absorption strength of the target, the transition of the optimal velocity becomes either continuous or discontinuous, which can be understood based on the Landau approach. In addition, we obtain the phase diagram indicating the passive-efficient and the active-efficient regions.

# Integrated method for identifying the optimal descriptor of acute critical illness: Development of septic infection related risk index (SIRRI) and investigation into patient's fate dynamics along SIRRI

**Ji-Hyun Kim**

*Creative Research Initiative Center for Chemical Dynamics in Living Cells, Chung-Ang University; Seoul 06974, Republic of Korea.*

Acute critical illnesses, particularly sepsis, pose significant challenges due to their sudden life-threatening nature and heterogeneous pathologies, demanding early detection and appropriate treatment. The lack of golden standards for early sepsis diagnosis has led to the exploration of deep learning (DL) methods for diagnostic or prognostic purposes, despite their opaque decision-making processes. Here, we propose a systematic and transparent method that integrates a DL module for early sepsis diagnosis, an explanation module for assessing feature importance and selecting key features, and a module for constructing multidimensional spaces defined by features generated through the application of mathematical operators to the identified features. Using this integrated method, we establish a septic infection-related risk index (SIRRI), composed only of six infection or inflammation-related biomarkers, as the optimal descriptor characterizing the severity of pathology in sepsis patients. In addition, we develop a prognosis model based on a set of multi-stage reaction-diffusion equations in SIRRI coordinates, enabling the quantitative prediction of time-dependent mortality or recovery rates of sepsis patients based on their SIRRI values at the onset of sepsis, with applicability across multiple datasets. These results demonstrate the utility of SIRRI as a novel effective biomarker for both diagnosis and prognosis in clinical practice, with potential applications extending beyond sepsis to other acute critical illnesses.

# Classical and quantum thermodynamics in a non-equilibrium regime: Application to Stirling engine

**Yoshitaka Tanimura**

*Kyoto University*

We develop a thermodynamic theory in the non-equilibrium regime by extending a theory based on the dimensionless (DL) minimum work principle previously developed for a thermodynamic system-bath model [S. Koyanagi and Y. Tanimura, http://arxiv.org/abs/2405.16787)]. Our results are described by non-equilibrium thermodynamic potentials expressed in time-derivative form in terms of extensive and intensive variables. This is made possible through the incorporation of waste heat, which is equivalent to the loss work consumed by the bath, into the definitions of thermodynamic potentials in a non-equilibrium regime. These potentials can be evaluated from the DL non-equilibrium-to-equilibrium minimum work principle, which is derived from the principle of DL minimum work and is equivalent to the second law of thermodynamics. We thus obtain the non-equilibrium Helmholtz-Gibbs potentials as free energies. Our results are verified numerically by simulating a Stirling engine consisting of two isothermal and two thermostatic processes using the quantum Fokker-Planck equations and the classical Kramers equation derived from the thermodynamic system-bath model. We then show that any thermodynamic process can be analyzed using a non-equilibrium work diagram analogous to the equilibrium one for given time-dependent intensive variables. The results can be used to develop efficient heat machines in non-equilibrium regimes.

# Universal Transport Distribution in Percolation

**Hyun Woo Cho**

*Department of Fine Chemistry*
*Seoul National University of Science and Technology (Seoultech)*

Transport phenomena arising from the emergence of infinite-sized clusters exhibit universal critical behaviors. Percolation theory has long been used to describe such critical phenomena, focusing mainly on average behaviors. However, the extension of these universal characteristics from average quantities to their distributions still remains an open question. In this presentation, we examine the electrical conductivity of percolating clusters in both continuum and lattice spaces to establish and characterize the universality of transport distributions in percolation. We observe a universal crossover in the distribution shape of transport properties from Gaussian to non-Gaussian near the percolation threshold, attributed to significant finite-size effects driven by the growing correlation length of the percolation cluster. Interestingly, at the percolation threshold, the non-Gaussian transport distributions exhibit universal finite-size scaling, governed by a transport exponent that determines the universality class of average transport. This finding indicates that both the average and the distribution of transport properties belong to the same universality class, governed by a shared universal principle with the same transport exponent. Our findings offer insights into universal feature in the distributions of various transport phenomena mediated by percolating clusters, opening novel avenues for characterizing transport across a broad spectrum of percolation-based systems.

# S6-3

## Algebraic techniques for quantum computing in quantum chemistry

**Artur Izmaylov**

*University of Toronto*

Quantum chemistry problem is one of the attractive targets for demonstrating quantum advantage of quantum computing technology. Having strongly correlated systems as the main target, I would like to discuss what new classical computing techniques need to be developed to help quantum computing algorithms to solve the electronic structure problem. Encoding the electronic Hamiltonian in the second quantized form on a quantum computer is not a trivial problem, and its efficiency can become a bottleneck for the entire quantum solution. Dealing with this Hamiltonian can be facilitated by partitioning it into a sum of fragments diagonalizable using rotations from either small Lie groups or the Clifford group. These fragments are convenient for performing various algebraic manipulations required in circuit compiling and quantum measurement. I will illustrate how the Hamiltonian partitioning can be used to improve performance of several quantum algorithms for quantum chemistry (e.g. Variational Quantum Eigensolver and Quantum Phase Estimation).

# Perfect Matching with Photons, Phonons, Electrons, and Spins

**Joonsuk Huh**

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In the near future, we will be able to use quantum technologies to simulate classically challenging molecular problems. Recent studies on quantum sampling have demonstrated that the corresponding restricted quantum computers are effective. Undoubtedly, the next phase of advancement in chemistry would be the quantum simulation of chemical systems. In 2015, a theoretical proposal [1] was put forward for quantum optical sampling with Gaussian light for molecular vibronic transition. Since then, several efforts [2] have been made to solve the molecular problem using different quantum platforms such as trapped-ion, superconducting circuits, and optics. In our attempt to simulate the molecular problem, we calculate Franck-Condon factors within a harmonic approximation. Different names in different contexts may refer to these factors, such as multivariate normal moments, multivariate Hermite polynomials, loop hafnian, and Kekulé structures. The problem may also be viewed from a graph interpretation perspective, corresponding to a counting problem of perfect matching a graph with loops. This interpretation is a powerful tool in understanding the problem's structure and complexity [3,4].
In my presentation, I will explore the fascinating world of quantum particles, including photons, phonons, electrons, and spins, and illustrate their identical mathematical structure. Through the problem's symmetries, I will show the beautiful connections between these platforms for practical molecular applications of these quantum tools.

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# Towards Quantum Force Fields Using Quantum Charged Oscillators

**Alexandre Tkatchenko**

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Quantum Charged (or Drude) Oscillators (QDOs) [1,2] offer a fundamental framework for future fully quantum atomistic force fields. In this talk, I will first review the concepts and theory behind coupled QDOs and the many-body dispersion (MBD) method [2,3] in particular. Then, I will demonstrate how the QDO/MBD framework is applicable to describe interatomic induction, dispersion and exchange interactions [4,5]. Finally, recent extensions to describe interatomic vdW potentials at all distances and even covalently-bonded dimers will be shown [6,7,8]. These results, taken together, elucidate the high promise of the coupled QDO framework as a fully quantum atomistic force field that can be developed as a community effort.

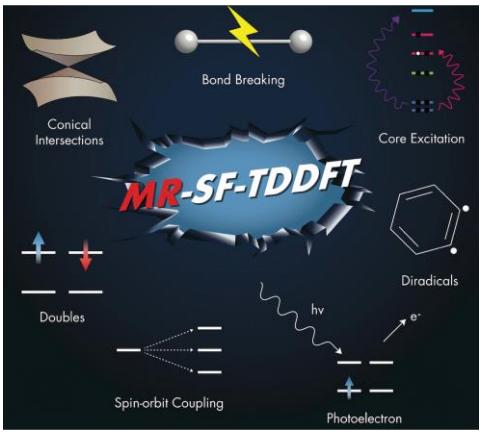
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# MRSF-TDDFT: A Breakthrough for DFT/TDDFT

**Cheol Ho Choi**

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The density functional theory (DFT) and linear response (LR) time-dependent (TD)-DFT are of utmost importance for routine computations. However, the single reference formulation of DFT is suffering from the description of open-shell singlet systems such as diradicals and bond-breaking. LR-TDDFT, on the other hand, finds difficulties in the modeling of conical intersections, doubly excited states, and core-level excitations. In this talk, we demonstrate that many of these limitations can be overcome by recently developed mixed-reference (MR) spin-flip (SF)-TDDFT1, providing an alternative yet accurate route for such challenging situations. Empowered by the practicality of LR formalism, it is anticipated that MRSF-TDDFT can become one of the major workhorses in general routine tasks.




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# Organic Synthesis Predictions Enabled by AI

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Reliable prediction of chemical reactivity remains in the realm of knowledgeable synthetic chemists. Automating this process by using artificial intelligence could accelerate synthesis design in future digital laboratories. While several machine learning approaches have demonstrated promising results, most current models use language models which is difficult to interpret and deviate from how human chemists analyze and predict reactions based on electronic changes. In this talk, I will talk about our recent efforts to learn organic reactivity based on chemical rules and algorithms. The issues related to the current reaction datasets and hence the importance of data curation to further improve the models will be discussed. I will then propose a new organic synthesis prediction AI methodology that can predict the reaction mechanisms with various chemical conditions.

# Magnus Expansion for Quantum Dynamical Processes

**Seogjoo J. Jang**

*Department of Chemistry and Biochemistry, Queens College, City University of New York & PhD Programs in Chemistry and Physics, Graduate Center, City University of New York*

For driven quantum dynamical processes such as in quantum control and quantum sensing, accurate dynamics calculation of quantum systems driven by time dependent Hamiltonian is essential. However, efficient implementations of such calculations are in general challenging and may incur artifacts if not done correctly. Magnus expansion provides a formally superior starting point in this respect since any finite truncation approximation remains unitary. I will present simple and straightforward general quantum propagators based on the Magnus expansion we have recently developed, and their applications for driven closed and open system quantum dynamics calculations.

# ABSTRACTS OF POSTERS

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| 2 | Xiangsong Cheng | Peking University | New Insights into Phase Space Representations for Finite-State Quantum Systems and Applications in Nonadiabatic Transition Dynamics |
| 3 | Yongin Cho | Seoul National University | Estimation of Differentiable Free Energy Profile from Multiple Equilibrium States Data via a Physics-Informed Energy-Based Model : Methods and Application to Thermodynamics of Water Density Fluctuations |
| 4 | Kwang Hyun Cho | Pohang University of Science and Technology | Effective harmonic oscillator model for excited state energy fluctuations in light harvesting complex |
| 5 | HyeonSik Choi | Seoul National University | Modeling Charge Transport in OLED Materials Using Multiscale Computational Chemistry Methodology |
| 6 | Seyong Choi | Pusan National University | VSFG spectrum of the Interfacial Water on a Solid Surface with Neural Network Potential |
| 7 | Yugon Eom | Pusan National University | Applications of Alchemical Free Energy Methods in Protein Interactions |
| 8 | Maryam Farmani | Kyungpook National University | Photochemistry of Thymine in Solution and DNA Revealed by an Electrostatic Embedding QM/MM Combined with Mixed-Reference Spin-Flip TDDFT |
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| 12 | Byeongjae Kim | Yonsei University | Determinant of successful basis set extrapolation of HF-DFT |
| 13 | Dong Geon Kim | Sungkyunkwan University | Lithium-ion diffusion mechanism in grain boundaries of Li6PS5Cl solid electrolytes using ab initio machine learning potential |
| 14 | Ingyeong Kim | The Catholic University of Korea | Theoretical Investigation of Reaction Mechanism on Formation of 1,2-Oxazetes |
| 15 | Jaewook Kim | Korea Institute of Science and Technology Information | Design principles for robust blue phosphorescent dye for long-lasting OLEDs |
| 16 | Jaeyoung Kim | Pusan National University | Molecular Dynamics Simulation of Visfatin-Derived Small Peptide with Angiogenic Activity |
| 17 | Jeongtae Kim | Seoul National University of Science and Technology | Thermal Conductivity of Super-cooled liquids |

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| 23 | Alireza Lashkari Pour | Kyungpook National Univeristy | Delayed Fluorescence from Inverted Singlet and Triplet Excited States in Heptazine Analogues HzT-FEX2 Studied by Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) |
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| 25 | Jay-Hak Lee | Seoul National University | Exploring Dynamical Phase Transitions in Spin-Lattice Models using the Double Bias Trajectory Ensemble Method |
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| 30 | YeongKyu Lee | KIAS | Electric Double Layer in Ionic Liquids: A Result of Interplay between Coupling Effects and Phase Demixing |
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| 32 | Mohsen Mazaherifar | Kyungpook National University | Optimizing Multiple ERI Tensor Contractions in Quantum Chemistry Using Hybrid MPI-OpenMP Approaches |
| 33 | Eunji Park | The Catholic University of Korea | Quantum chemical calculations of electron affinities of alkaline earth metal atoms (Ca, Sr, Ba, and Ra) |
| 34 | Jeongmin Park | The Catholic University of Korea | Multireference Configuration Interaction including Spin-Orbit Coupling Study of Potential Energy Curves of gold monotelluride (AuTe) and Energy Levels of Te atom |
| 35 | Joohyeong Park | Seoul National University of Science and Technology | Universal Scaling Laws for the Interfacial Thickness of Polymer Globules |

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| **36** | Taehyeon Park | Sungkyunkwan University | Uncertainty Quantification of Bayesian Deep Learning ab initio Potential |
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| **45** | Chou-HsunYang | Academia Sinica | Non-negligible outer-shell reorganization energy for charge transfer in nonpolar systems |
| **46** | Hyeonseok Yang | Kyoto University | Aharonov-Bohm effect at Finite temperature |
| **47** | Ji Woong Yu | KIAS | Spatio-Temporal Characterization of Water Diffusion Anomalies in Saline Solutions Using Machine Learning Force Field |

**P-01**

# Semi-classical path integral simulations to understand the decoherence of a qubit in a structured environment

**Chirag Arora, David F. Coker***

*Department of Chemistry, Boston University, USA*

In the era of emerging quantum technologies and the dream to utilize the 'quantum advantage' to speed up computationally daunting tasks, it remains fundamentally important to study and clearly understand the various possible control knobs for qubit decoherence. This is because every practically usable quantum system is essentially an open quantum system and system-bath entanglement is inescapable. Understanding how the system entangles with the bath can potentially serve as a motivation to come up with clever design principles to mitigate decoherence. Although, several control strategies such as use of shaped electromagnetic (EM) pulses, feedback loops etc. have both been theoretically proposed and experimentally demonstrated to alter the quantum dynamics of a qubit interacting with its bath (environment). The nature of the effect a structured bath on the decoherence of qubit is seldom explored.

In this work, we derive an analytic expression for the thermalized Wigner density of a two-level bath[3]. Semi-classical path integral simulations within the partially linearized density matrix (PLDM) formalism [1] are then employed to study qubit decoherence in a bath of two-level systems. Recent theoretical work [2] using a related path-integral based quantum dynamics methodology has shown that in a harmonic bath, low-frequency bath modes entangle strongly with a qubit. Our work builds upon this study and explores the qubit-bath entanglement entropy in this structured bath setup. A two-level quantum system can be described by Pauli spin matrices and thus ascribed a fictitious 'spin'. This work will serve as a steppingstone to study true Fermionic baths, specifically, a spin-Fermion model (a natural extension of the spin-Boson problem). Recent work exploring how boson operators can mimic Fermionic structure and dynamics [4] will be extended to enable this study. Practically, such a bath structure is of relevance to many emerging areas of quantum technologies such a single molecule circuits, molecular magnonics, and quantum electrochemistry where consideration of both Bosonic and Fermionic degrees of freedom become important.

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**P-02**

# New Insights into Phase Space Representations for Finite-State Quantum Systems and Applications in Nonadiabatic Transition Dynamics

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Chemical systems often consist of both electronic and nuclear degrees of freedom. fstates, electronic degrees of freedom are typically treated as finite-state quantum systems. The study of dynamics of finite-state quantum systems is instrumental in better understanding nonadiabatic transitions in systems such as light-harvesting complexes and elementary chemical reactions.
For two-state quantum systems, we propose a class of phase space isomorphic representations for exact population dynamics. It utilizes positive semi-definite non-covariant phase space functions, time-dependent weight functions on constraint phase space, and time-dependent normalization factors. The triangle window function approach proposed in *J. Chem. Phys.* **2016**, **145**: 144108 leads to its special case. For general finite-state quantum systems, we introduce novel phase space representations incorporating triangle window functions for exact electronic dynamics involving electronic coherence terms. When these representations for finite-state systems are combined with the recently developed nonadiabatic field (NaF) dynamics, we achieve satisfying computational results in various models of nonadiabatic chemical systems.

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# P-03

# Estimation of Differentiable Free Energy Profile from Multiple Equilibrium States Data via a Physics-Informed Energy-Based Model: Methods and Application to Thermodynamics of Water Density Fluctuations

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We present an energy-based generative model approach to optimize differentiable free energy profile from samples obtained across multiple equilibrium states. First, we rederive the multistate Bennett acceptance ratio method as a Bayes predictor for a classification problem. Driven by this perspective, we transform the free energy estimation problem into learning an energy-based generative model within an extended configurational space. Here the interaction energy terms between the collective variables and the control parameters are informed by the simulation bias potential. This approach allows simultaneous optimization of a differentiable, physically parameterized free energy function for both the collective variables and the control parameters. Finally, we validate the estimator by analyzing enhanced sampling data for water density fluctuations and apply it to support an improved model of water density fluctuation thermodynamics.

**P-04**

# Effective harmonic oscillator model for excited state energy fluctuations in light harvesting complex

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We propose a tactic to construct a minimal harmonic bath that represents environmental effects on the quantum subsystem, and utilize it to simulate the energy transfer process in the light harvesting 2 (LH2) complex. Traditionally, the harmonic bath is derived from normal mode analysis. However, we found that anharmonicity, often ignored in normal mode analysis, leads to variations in the vibrational frequency of each normal mode, posing challenges in determining frequencies and consequent vibronic couplings. Instead, we optimized the vibrational frequencies and vibronic couplings to replicate the results of the all-atomistic simulations. As a result, we obtained a set of underdamped harmonic oscillators that model the intramolecular vibrations, with an overdamped phonon band representing the intermolecular contributions. By employing this simplified bath and a mixed quantum-classical method, we demonstrated the energy transfer process within the LH2 complex with explicit non-equilibrium dynamics of each oscillator. This harmonic bath model, clearly connected to the atomistic system, can provide insights into the molecular mechanisms underlying the efficient energy transfer process

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# P-05

# Modeling Charge Transport in OLED Materials Using Multiscale Computational Chemistry Methodology

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OLED material research utilizes a screening procedure involving the synthesis of numerous potential materials, followed by an analysis to identify suitable molecules. This in-silico approach not only offers cost-effectiveness but also provides a fresh perspective for examining properties from a microscopic standpoint. Simulating OLED materials necessitates simulations across various length and timescales. While previous studies employed the Gaussian distribution model and Miller-Abrahams rate equation for simulation, our objective being the prediction of properties solely from molecular structure led us to employ the Marcus rate equation, which requires fewer prefactors. Our method incorporates the image charge method into the site energy calculation necessary for the Marcus rate equation. Additionally, we introduce a mapping method to construct a lattice model from molecular dynamics morphology, crucial for computing site energies while retaining information about dipole moments and transfer integrals. Mobility calculations for 11 molecules correlate well with experimental values. We observe that charge carriers predominantly become trapped in a few molecular sites for most of the time without the application of an electric field. Consequently, our approach enables the development of models capable of tracing trajectories in multi-charge and multi-layer scenarios.

P-06

# VSFG spectrum of the Interfacial Water on a Solid Surface with Neural Network Potential

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Structurally ordered layers of water are universally formed on a solid surface in an aqueous solution or under ambient conditions. Such an ordered layer, called a hydration layer, significantly affects the wetting of a surface and the freezing process involving heterogeneous nucleation. Interestingly, a hydration layer develops not only on a hydrophilic but also on a hydrophobic surface.

Vibrational sum frequency generation (VSFG) spectroscopy, which has the high interface selectivity, is one of the methods to probe the molecular structure of a hydration layer. With VSFG spectrum, it can be possible to analyze the anisotropic orientation, chemical bonds, especially hydrogen bonds, and ultrafast dynamics including OH bond stretching of the water molecules in a hydration layer. However, obtaining the spectra form simulation requires significant large computational resources.

To overcome this limitation, we applied the machine learning technique called neural network potential. This approach significantly reduces the computational cost while maintaining high accuracy in simulating the VSFG spectrum. Our results demonstrate the effectiveness of neural network potentials in efficiently probing the structural and dynamic properties of hydration layer on the α-SiO2 surface. This advancement paves the way for more detailed and extensive studies of interfacial water using computationally efficient methods.

P-07

# Applications of Alchemical Free Energy Methods in Protein Interactions

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Since the emergence of computational methodologies such as molecular dynamics (MD) simulations, the simulation methods have been serving as a complementary tool for wet-lab experiments. In recent years, MD simulations have been increasingly incorporated into various research fields, with protein and drug research benefiting substantially. One of the most utilized methods among the computational investigations is alchemical free energy methods, which enable the prediction of binding affinities between proteins and small molecules. Here we suggest two applications of alchemical free energy methods across diverse protein systems.

The first topic is the computational investigation of the thermodynamic stability of an oxygen molecule within the maltose-binding protein (MBP). MBP is a metabolic enzyme responsible for the utilization of maltose and maltodextrins. A recent experiment revealed that MBP can serve as a scaffold that contributes to the generation of reactive oxygen species, resulting in the intracellular accumulation of oxidative stress. We conducted free energy calculations on the MBP-$O_2$ complex and found out that the binding free energy difference between MBP and the $O_2$ molecule was negligible, within the thermal energy at room temperature.

Secondly, we applied the alchemical methods to engineer the binding affinity of green fluorescent protein (GFP) through single-point mutations. GFP has been used as one of the most effective agents for fluorescence microscopy, and it exhibits weak homodimerization at high concentrations. We utilized a machine-learning method and the alchemical approaches to systematically mutate the interface of GFP homodimers and predict the binding affinity change upon each mutation. The results demonstrated that both the machine-learning method and the MD simulations had an overall correlation in predicting binding affinities of GFP.

We expect our study to broaden the applications in the calculation of binding energies according to various protein interactions. Specifically, our methods can be applied to the optimization of lead compounds in drug discovery and the prediction of the effects of disease-induced mutations in protein folding and binding.

**P-08**

# Photochemistry of Thymine in Solution and DNA Revealed by an Electrostatic Embedding QM/MM Combined with Mixed-Reference Spin-Flip TDDFT

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The photochemistry of nucleobases, important for their role as building blocks of DNA, is largely affected by the electrostatic environment in which they are soaked. For example, despite the numerous studies of thymine in solution and DNA, there is still a debate on the photochemical deactivation pathways after UV absorption. Many theoretical models are oversimplified due to the lack of computationally accurate and efficient electronic structure methodologies that capture excited state electron correlation effects when nucleobases are embedded in large electrostatic media. Here, we combine mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT) with electrostatic embedding QM/MM using electrostatic potential fitting fitted (ESPF) atomic charges, as a strategy to accurately and efficiently describe the electronic structure of chromophores polarized by an electrostatic medium. In particular, we develop analytic expressions for the energy and gradient of MRSF/MM based on the ESPF coupling using atom- centered grids and total charge conservation. We apply this methodology to the study of solvation effects on thymine photochemistry in water and thymine dimers in DNA. In the former, the combination of trajectory surface hopping (TSH) nonadiabatic molecular dynamics (NAMD) with MRSF/MM remarkably revealed accelerated deactivation decay pathways, which is consistent with the experimental decay time of ~400 fs. The enhanced hopping rate can be explained by the preferential stabilization of corresponding conical interactions due to their increased dipole moments. Structurally, it is a consequence of characteristic methyl puckered geometries near the conical intersection region. For the thymine dimer in B-DNA, we found new photochemical pathways through conical intersections that could explain the formation of cyclobutadiene dimers and 6−4 photoproducts.

# Phase Space Functions for Trajectory-Based Nonadiabatic Field Dynamics

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The Liu group has developed phase space functions within the constraint coordinate-momentum phase space (CPS)[1-3] framework for finite-state quantum systems. Recently, it was revealed that the triangle window (TW) [4-5] approach provides an isomorphic representation of the exact population-population correlation function of the two-state systems. By utilizing both TW phase functions and CPS phase functions, we have formulated a novel representation of discrete electronic degrees of freedom (DOFs)[5,7]. When combined with nonadiabatic field (NaF) dynamics[6], this new approach, termed NaF-TW[7], is capable of faithfully capturing the dynamical interplay between electronic and nuclear DOFs in both the condensed-phase and gas-phase scenarios. Compared to the symmetrical quasi-classical (SQC) method[4], NaF-TW not only ensures the positive population dynamics, but also significantly outperforms in cases where the bifurcation characteristic of nuclear motion in the asymptotic region is important[7]. The NaF-TW method is promising for offering new reliable and effective tools in understanding and predicting important nonadiabatic transition phenomena, including photo-chemistry reactions, light-driven and electron/hole transfer processes.

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**P-10**

# Universality of Electrical Conductivity Distribution in Percolation

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In this work, we investigate the distribution of electrical conductivity in percolating clusters of hard spheres within both continuum and lattice frameworks. By randomly distributing hard spheres without overlap, we generate percolating clusters and use the finite size scaling method to determine the precise volume fraction of hard spheres ($\phi_c$) at which percolating clusters begin to emerge. We find that not only the average electrical conductivity of the percolating clusters exhibits universal scaling behaviors, but its distribution also conforms to a universal non-Gaussian shape. This non-Gaussian distribution shows universal finite-size scaling, governed by a transport exponent that also defines the universality class of average transport. Interestingly, this universal non-Gaussian distribution transforms into a Gaussian distribution as $\phi$ increases beyond $\phi_c$. We demonstrate that this shift in distribution shape occurs at the volume fraction where the correlation length of the percolating cluster is comparable to the system size, indicating that the universal non-Gaussian distribution of transport properties in percolating clusters is linked to the critical behaviors associated with the growing length scale of the percolating cluster.

# Effects of Energetic Disorder in Doped Conducting Polymer: Molecular Dynamics and Monte Carlo Study

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Applying dopants in organic semiconductors has been suggested as a convenient and powerful method to increase their electrical conductivity[1]. In such processes aimed at enhancing performance, understanding the underlying principles of doping plays a crucial role[2]. Among the various factors affecting electrical conductivity, the intrinsic energetic disorder of organic semiconductors has recently garnered significant attention[3,4]. However, limited theoretical or experimental characterization of their quantitative contributions to the overall conductivity has hindered molecular understanding of the underlying mechanism.

In this study, theoretical approaches were employed to investigate how intrinsic energetic disorder affects conductivity. Initially, regioregular and regiorandom P3HT(Poly(3-hexylthiophene-2,5-diyl)) with $FeCl_3$ dopant molecules were modeled to simulate disordered organic semiconductor structures using molecular dynamics simulations. Subsequently, Metropolis Monte Carlo simulations were conducted to elucidate the relationship between Coulombic hole-anion interaction. Finally, kinetic Monte Carlo simulations for electron transfer were implemented to determine charge carrier mobility and transport energy of holes. Specifically, proposing the random movement of holes with charge transfer rates related to semiclassical Marcus theory[5,6] and transition state theory[6,7] facilitated the realistic modeling of the charge transfer process. Through these methods, we investigated the effects of intrinsic energetic disorder in organic semiconductors on each of the main processes

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P-12

# Determinant of successful basis set extrapolation of HF-DFT

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Basis set extrapolation aims to minimize the error arising from the use of finite basis sets, which lead to an inaccurate description of wavefunctions or electron densities. While basis set extrapolation attempts to obtain results at the Complete Basis Set (CBS) limit, this method has the advantage of reducing computational cost, as the CBS limit is achieved by extrapolating from smaller basis set results.

Hartree-Fock (HF) DFT is a scheme that replaces the self-consistently (SC) calculated density with the HF density when the SC density is physically inaccurate. HF-DFT has the potential to reduce density-driven errors by mitigating electron delocalization and self-interaction errors.

In this study, we combine HF-DFT with basis set extrapolation and analyze the rationale behind the successful extrapolation of HF-DFT. By closely examining electronic structures, we found that successfully extrapolated systems exhibited consistent electron density, orbital structures, and spin densities across basis sets. Systems that failed to extrapolate correctly showed deviations from the consistency of electronic structures.

# P-13

# Lithium-ion diffusion mechanism in grain boundaries of $Li_6PS_5Cl$ solid electrolytes using ab initio machine learning potential

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$Li_6PS_5C$ (LPSC) is an argyrodite-type sulfide-based solid electrolyte. Making solid electrolytes usually involves mixing raw materials mechanically (or milling), then heating them to high temperatures to form a glass (or melting), and finally crystallizing them (annealing, sintering). During this process, many nanocrystals form, and we wanted to study the grain boundaries(GBs) between them. We made GB models using the $Li_6PS_5Cl$ model, which belongs to the $F\bar{4}3m$ space group.[1] Since these GB models have thousands of atoms, regular Density Functional Theory(DFT) Molecular Dynamics(MD) calculations can be very slow and challenging. To solve this, we created a dataset using unit cell and 2x2x2 supercell DFT-MD calculations with VASP(Vienna Ab initio Simulation Package)[2] and trained a Machine Learning Potential(MLP) using E3NN[3] with this dataset. We then used the MLP to perform MD calculations on LPSC GB models with thousands of atoms. We aim to analyze the results to study properties the density of states(DOS) and diffusion coefficients of Li-ions in GB models.

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**P-14**

# Theoretical Investigation of Reaction Mechanism on Formation of 1,2-Oxazetes

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1,2-Oxazetes are a class of five-membered heterocyclic rings with adjacent oxygen and nitrogen atoms. Although the synthesis has recently succeeded [1], the exact reaction mechanism has not yet been clarified. These compounds are attracting significant interest in organic chemistry due to their unique multi-step synthesis pathways and potential applications. Hence, we have investigated the reaction mechanism of the formation of 1,2-oxazete from cedrene. This study elucidated the reaction mechanism using density functional theory (MN15) with large-size basis sets. In addition, single-point energy calculations were conducted utilizing domain-based local pair natural orbital coupled-cluster singles and doubles with perturbative triples (DLPNO-CCSD(T)), yielding accurate energetic values and thereby facilitating the derivation of a highly reliable mechanism.

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**P-15**

# Unveiling thermal and electrical degradation pathways for chemically robust blue OLED material design

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The short lifetime of blue organic light-emitting diodes (OLEDs) remains a significant challenge. This short lifetime is often attributed to degradation reactions initiated by high-energy excitons generated inside the device. This explanation effectively accounts for the short lifetime of blue OLEDs compared to red or green devices. However, to increase the lifetime of blue OLED devices, it is necessary to address the inherent vulnerabilities of OLED materials. In this presentation, we present methods to investigate the chemical reactions that OLED materials can undergo, with a focus on their thermal and electrical stability. First, we investigated thermal degradation reactions that can occur during device fabrication. A combined computational and mass spectrometry approach is presented to elucidate these pathways.[1] Second, we investigated the electron-induced degradation reactions of blue phosphorescent dyes during device operation. Through quantum chemical calculations and device degradation experiments, we demonstrate the critical role of electron-induced reactions in the short lifetime of blue OLEDs.[2]

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**P-16**

# Molecular Dynamics Simulation of Visfatin-Derived Small Peptide with Angiogenic Activity

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Angiogenesis plays an important role in female reproduction including development of follicles and implantation. Visfatin which is secreted from various tissues not only enhances the expression of vascular endothelial growth factor (VEGF), but also exhibits angiogenic effect itself. Previous we designed visfatin-derived small peptides which mimic angiogenic activity of visfatin using computer-aided drug design techniques. In this study, we used all-atom molecular dynamics (MD) simulation to investigate the interaction of visfatin-peptide complex. Interaction fingerprint was extracted from our MD simulation trajectories, and umbrella sampling method was implemented to calculate binding energy of visfatin-peptide.

**P-17**

# Thermal Conductivity of Super-cooled liquids

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Understanding the thermal transport of glass-forming liquids is crucial for elucidating the physical origins of the glass transition and developing efficient thermoelectric materials and coolants. In this study, we investigate the temperature dependence of the thermal conductivity of glass-forming liquids using Molecular Dynamics (MD) simulations. We employ the Kob-Andersen (KA) binary liquids as a model system and calculate the thermal conductivity $\lambda$ at various temperatures T using the Green-Kubo (GK) formalism. Our results show that as T decreases below the onset temperature $T_{on}$, the structural relaxations of KA liquids become sluggish, leading to subdiffusive regimes in the mean-squared displacement and a clear separation between $\alpha$ and $\beta$ relaxations in the intermediate scattering functions. Despite these changes, $\lambda$ consistently follows a scaling relation with T, specifically $\lambda \sim T^{\frac{1}{4}}$ across all temperature ranges. We find that the auto-correlation function of the heat flux in the GK formalism vanishes over a very short time scale compared to the structural relaxation time, indicating that heat conduction occurs over short time scales associated with local dynamics and structures. This may explain why the temperature dependence of thermal conductivity is minimally affected by the long-time scale structural relaxation of glassy liquids.

# Revisiting the global minimum of $Au_{10}$ clusters

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The investigation of gold clusters has garnered significant attention due to their catalytic properties hinging on size and molecular structures. A large number of previous studies have been conducted to identify the crossing point from planar to three-dimensional structures. Still, the results remain unclear because of the varying density functionals and basis sets used. Therefore, this study aims to determine the global minimum of the neutral $Au_{10}$ structure using high-level quantum chemical methods. We primarily employed density functional theory (DFT) as the main tool for our investigation. Among various DFT functionals (LC-BLYP, PBE, TPSS, revTPSS, B1B95, and TPSSh) used with the dhf-QZVPP basis set, B1B95 demonstrated the closest performance to the coupled-cluster singles and doubles with perturbative triples (CCSD(T)) method when comparing relative energies (ΔEs). Additionally, we conducted two-component spin-orbit DFT (SODFT) calculations to examine the effect of spin-orbit coupling (SOC) on the molecular properties of $Au_{10}$ isomers. Most previous studies didn't account for the SOC effect owing to the electron configuration of Au being $5d^{10}6s$, but SOC could significantly affect results when $6p$ orbitals of Au are involved. We propose a straightforward diagnostic method to determine the influence of SO effects on the relative energies of $Au_{10}$ clusters.

**P-19**

# Molecular Dynamics Simulation Study about Deformation of HFC-23 Hydrate

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Gas hydrate is a type of icy crystalline clathrate. It traps guest molecules in polyhedral cages formed by hydrogen-bonded water molecules under low temperature and high-pressure conditions. Methane hydrate, which houses methane gas as the guest molecule, is the most abundant type. Recently, researchers have been exploring the potential of using the structure and characteristics of gas hydrates in fire extinguishing agents (HFC-23, HFC-125, etc.) to suppress various types of fires, such as wildfires, skyscraper fires. Fire extinguishing agent hydrates should possess various characteristics like stability under atmospheric conditions, crystal melting speed, and anti-agglomerant properties. Although many experimental and computational studies have been conducted on methane or carbon dioxide in previous gas hydrate research, hydrate studies on extinguishing gases are not widely reported. In this study, we performed a thermodynamic analysis of hydrate decomposition through Potential of Mean Force (PMF), examining the departure of guest molecules in fire extinguishing agent hydrates using restrained Molecular Dynamics (MD).

# Navigating Density Sensitivity Behaviour Across Functional Rungs

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Density Functional Theory (DFT) is a quantum computational method that achieves a balance between computational efficiency and accuracy, making it widely used in many fields today. However, DFT can suffer from density-driven errors, which occur when it produces an incorrect electron density. Density-Corrected Density Functional Theory (DC-DFT) addresses this issue by using an alternative density rather than the self-consistent one generated by DFT. An example of this approach is HF-DFT, which employs the Hartree-Fock (HF) density. Identifying these density-driven errors necessitates the exact density, a task complicated by the numerical challenges of Kohn-Sham (KS) inversion. Density sensitivity is a critical metric that evaluates how changes in density influence both the energy calculations of the system and the functionals used. This sensitivity can help determine the potential for reducing density-driven errors with HF-DFT. Although density sensitivity may vary with different functionals, there is limited understanding of this variation. This study aims to investigate the relationship between density sensitivity and various properties depending on the functional rung.

# Property-networking deep learning model for materials with an artificial intelligence

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As the demand for precise predictions of materials properties grows alongside the rapid pace of data-driven materials discovery, there's a pressing need to advance artificial intelligence technologies. These technologies must not only expand materials databases beyond density functional theory (DFT) but also develop deep learning (DL) models capable of accurate predictions with limited high-fidelity data.

To address this issue, we developed a new DL model named PRoperty-networking Orbital Field maTrix-convolutional Neural Network (PROFiT-Net). It utilizes a crystal structure representation based on the orbital field matrix (OFM), modified to integrate elemental properties and valence electron configurations. This unique representation captures intricate relationships within the crystal, enabling PROFiT-Net to achieve remarkable accuracy in predicting dielectric constants, experimental band gaps, and formation enthalpies compared to other leading DL models. Notably, our model avoids predicting unphysical negative band gaps and exhibits a Penn-model-like trend while remaining scalable. With these capabilities, we believe PROFiT-Net holds significant potential for accelerating the development of functional materials.

**P-22**

# The effects of the substituent to Photoisomerization of Norbornadiene

**Taekyeong Kim**, Cheol Ho Choi

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The molecular solar thermal (MOST) energy storage with the light-induced isomerization reaction of norbornadiene (NBD) to quadricyclane (QC) is a top candidate of the renewable and the sustainable energy source. It can store the energy in the new chemical bonds formed by the [2+2] cycloaddition reaction and it also has the high energy storage density and long thermal reversion lifetime. However, because of the high energy of absorption and the low quantum yield (QY) of QC, efficiency of the system could be limited without any work. There are a few ways to make the system efficient. The one way is the functionalization of the πcc bonds of NBD which red-shift the absorption However, it also increase the molecular weight, causing the decrease of the storage density [1]. Our results show that how different the vertical excitation energy and the absorption is depending on which substituent is bonded. We did calculation with various combination of functional and basis set.

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P-23

# Delayed Fluorescence from Inverted Singlet and Triplet Excited States in Heptazine Analogues HzT-FEX2 Studied by Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT)

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This study explores the photophysical properties of heptazine analogues, with a focus on HzT-FEX2, utilizing Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT). Heptazine derivatives are highly regarded for their exceptional stability and electronic properties, making them promising candidates for optoelectronic and photovoltaic applications. A deep understanding of the mechanisms behind their delayed fluorescence is essential for enhancing their performance in these fields. Our investigation into the singlet-triplet energy gap in heptazine analogues revealed that traditional methods using TDDFT like BHHLYP and B3LYP tend to overestimate this gap. In contrast, MRSF-TDDFT has proven to be a more efficient and accurate approach for studying these systems. To achieve optimal results, we also attempted to optimize the VAEE functional using MRSF-TDDFT.

# High-Throughput Screening of Dual Atom Catalysts with Machine Learning Global Optimization

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To mitigate the climate change, reducing carbon emission has become the most urgent agenda across the globe. As most of carbon emission is from fossil fuels, high performing electrocatalysts can be an alternative solution for sustainable energy source. Recently, dual atom electrocatalysts where metal dimers are ligated by $N_xC_y$ showed a great promise for hydrogen evolution(HER) and oxygen evolution/reduction reactions(OER/ORR) [1,2]. Compared to single atom catalysts [3], dual atom catalysts take advantages in having more tunability and structural/compositional diversity. Here, we perform high throughput screening of dual atom catalysts at density functional theory(DFT) level. As most of highly performing electrocatalysts are made of expensive rare metals (Pt/Ir/Ru), it is necessary to find an electrocatalyst, which is cheap and abundant. Therefore, we perform high-throughput screening of dual atom catalysts on $N_xC_y$ substrates using Machine Learning, focusing on transition metals from 3d and 4d series. We analyze data about electrocatalytic reactions. The ultimate goal is to investigate the HER and OER/ORR on these structures, exploring how the reactions mechanism occur and assessing their effectiveness as electrocatalysts [4].

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**P-25**

# Exploring Dynamical Phase Transitions in Spin-Lattice Models using the Double-Bias Trajectory Ensemble Method

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In this poster, we investigate non-equilibrium states using the trajectory ensemble method to explore various non-equilibrium states within two lattice models: the 1D Ising model and the kinetically constrained model (KCM). Specifically, we introduce a double bias ensemble incorporating conjugate fields $s$ and $g$, corresponding to dynamical activity and trajectory energy, respectively. Through analytical calculations and the multistate Bennett acceptance ratio (MBAR), we derive the dynamical free energy and examine the behavior of dynamical phase transitions within the ($s$,$g$,$T$) parameter space. Notably, in the Ising model, we observe a decoupling between activity and energy under specific non-equilibrium conditions, prompting an investigation into unique dynamical phases such as the antiferromagnetic phase and the freezing-by-heating phenomenon. Moreover, in the KCM, a coarse-grained glass model, we confirm the existence of dynamical phase transitions with varying $g$ fields and identify the conditions that trigger these transitions based on temperature variations facilitated by the introduction of both $s$ and $g$ fields. This research provides comprehensive insights into the dynamical phase transitions in spin-lattice models and highlights the unique behaviors arising from the far-from-equilibrium states.

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# Transport Dynamics of Water Molecules nanoconfined between lipid membranes

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Understanding of water behavior confined between biological membranes in nanoscale is crucial to elucidate various biological functions. The interfacial environment between the membrane and water plays a significant role in governing the dynamic properties of nanoconfined water. Despite extensive investigations into the dynamic properties of nanoconfined water, a quantitative understanding of the dynamic heterogeneity of water motion and its relationship with the interfacial environment remains elusive. In this study, we present a novel transport equation for water molecules in the intermembrane space [1], providing a quantitative explanation for molecular dynamics (MD) simulation results. Our findings reveal that the unique transport dynamics of water molecules comes from the fluctuations in the lateral diffusion coefficient, influenced by their longitudinal motion perpendicular to the membranes. Additionally, we identify an interfacial region where water exhibits unique physical properties, remaining unaffected by variations in the intermembrane distance.

[1] M. Lee *et al.*, Transport Dynamics of Water Molecules Confined between Lipid Membranes, *J. Phys. Chem. Lett* **2024,** 15, 16, 4437-4443.

**P-27**

# Resolving dispersion corrections with density-corrected DFT

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Almost all empirical parameterizations of dispersion corrections in DFT use only energy errors, thereby mixing functional and density-driven errors. We introduce density and dispersion corrected DFT ($D^2C$-DFT), a dual-calibration approach that accounts for density delocalization errors when parametrizing dispersion interactions. We simply exclude density-sensitive reactions from the training data. We find a significant reduction in both errors and variation among several semilocal functionals and their global hybrids when tailored dispersion corrections are employed with Hartree-Fock densities.

# Two Fates of Peptide Isomerization Kinetics near Aqueous Interfaces

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Peptides at the interface have been explored in diverse range of applications ranging from nanomaterials to biomedical applications. Especially, the molecular behavior of peptides at interfaces is deeply involved with the biocompatibility of a biomaterial such as biosensor, microelectronics, and antibody drugs. It is therefore crucial to examine the stability of molecular conformations and the transition rates between conformation near interfaces, which are expected to be different from that of bulk due to the loss of solvation free energy. The lack of appropriate techniques to investigate the molecular behavior near aqueous interfaces calls for the computational methods to elucidate the interfacial effects on peptide conformational equilibria and isomerization kinetics. In here, we leverage explicit-solvent classical MD simulation to elucidate the thermodynamic and kinetic behavior of solvated alanine dipeptide at aqueous interfaces (air-water, POPC-water, and octanol-water). Multidimensional free energy calculations show that the degree of stabilization near aqueous interfaces are different among conformations. Especially, the transition state TS1 that connects β(PPII, C5) state to αL state is relatively less stabilized at aqueous interfaces, whereas the transition state TS2 that connects β(PPII, C5) state to α state is relatively more stabilized at aqueous interfaces. Transition path sampling simulation combined with umbrella sampling (TPS+U) shows that the isomerization rate constant for β(PPII, C5) state to αL state transition is suppressed by three times, whereas that for β(PPII, C5) state to α state transition is enhanced by three times. Energy decomposition analysis reveals that the two fates of the peptide isomerization kinetics are governed by the amount of the loss of solvation free energy near aqueous interfaces. TS1 conformation is more accessible to solvents due to its compact nature, which leads to the high solvation energy penalty near aqueous interfaces. For the TS2 conformation, however, the solvent-inaccessible nature of N-methyl hydrogen drops the solvation energy at bulk, which leads to strong stabilization at aqueous interfaces due to less solvation energy penalty.

P-29

# Determining Active Sites through Density Sensitivity in Embedding Theory

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Density functional theory is efficient method for electronic structure calculations due to its low computational cost, but its moderate accuracy may require the use of more computationally expensive methods for accurate results in certain systems. For these systems, embedding theory can be used to achieve both accuracy and low cost. In the embedding theory, active sites are defined as important areas of the system and calculated using high-level methods. This reduces the cost while maintaining reliable accuracy. Since active sites have a greater influence on chemical properties such as energy, it is important to determine the correct active sites. However, it is not always straightforward to know which area has how much influence. While chemical intuition may be useful in some systems, it may not be applicable in others. In this study, we present an automated approach to determine active sites based on density sensitivity. The density sensitivity is used as an indicator of where chemical properties have more influence and is calculated before embedding using low-level methods. We have developed a method for calculating the density sensitivity of each area of the system and selecting orbitals based on their degree of localization. Our results demonstrate the reliability of this method.

# P-30

## Electric Double Layer in Ionic Liquids: A Result of Interplay between Coupling Effects and Phase Demixing

**YeongKyu Lee**

*KIAS*

Ionic liquids (ILs) are appealing electrolytes for their favorable physicochemical properties. However, despite their longstanding use, understanding the capacitive behavior of ILs remains challenging. This is largely due to the formation of a non-conventional electric double layer (EDL) at the electrode-electrolyte interface. This study shows that the short-range Yukawa interactions, representing the large anisotropically charged ILs, demix IL to create a spontaneous surface charge separation, which is reinforced by the strongly coupled charge interaction. The properties of the condensed layer, the onset of charge separation, and the rise of overscreening and crowding critically depend on the asymmetry of Yukawa interactions.

**P-31**

# Studying Dynamical Phase Transitions in Kinetically Constrained Models Using Energy-Activity Double Bias Matrix Product State

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*Department of Chemistry, Seoul National University, Seoul 08826, Republic of Korea*

In this study, we explore dynamical phase transitions in two representative kinetically constrained models—the 1D Fredrickson-Andersen and East Models—using a recently developed double-bias ensemble approach combined with tensor network techniques for the first time. We first confirm that tensor networks allow us to numerically approximate the large deviation statistics of dynamics by finding the leading eigenvalues of the tilted dynamical generators with double biasing fields. As concrete examples, we present phase diagrams in the (s, g, T) space obtained via tensor networks, which show good qualitative agreement with mean-field results and our previous extensive numerical simulations using the path sampling method. Additionally, we demonstrate that extensive finite-size scaling analysis can be performed under various (s, g, T) conditions using this method. Our study extends our previous understanding of scaling functions.

P-32

# Optimizing Multiple ERI Tensor Contractions in Quantum Chemistry Using Hybrid MPI-OpenMP Approaches

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In quantum chemistry, the contraction of multiple Electron Repulsion Integral (ERI) tensors with various matrices, known as Multiple ERI Tensor Contractions (METC), is a common and computationally intensive task. This process, particularly significant in response theories, can become a substantial bottleneck, often exceeding the computational demands of ERI calculations. These demands scale with the number of excited states and the kernel pre-factors, making the process computationally expensive. Optimizing METC performance can be achieved through several methods, including reformatting the data layout of interim density and Fock matrices, introducing an intermediate ERI quartet buffer, and optimizing loop ordering for higher cache hit rate. Applying a hybrid MPI-OpenMP environment can greatly enhance the performance of these methods. This hybrid approach utilizes MPI for distributed memory parallelism and OpenMP for shared memory parallelism, effectively leveraging modern multi-node and multi-core architectures. The hybrid model aims to balance the computational workload across all available resources, reduce communication overhead, and optimize memory usage. This approach demonstrates significant potential for enhancing performance in various quantum chemistry computations, providing a robust framework for future computational advancements in the field.

# P-33

# Quantum chemical calculations of electron affinities of alkaline earth metal atoms (Ca, Sr, Ba, and Ra)

**Eunji Park, Jeongmin Park, Ingyeong Kim, Jungyoon Kim, Wonil Seo, and Joonghan Kim***

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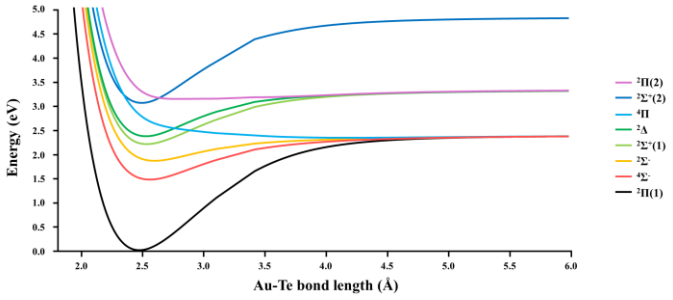
We performed high-level ab initio quantum chemical calculations, incorporating higher-order excitations, spin-orbit coupling (SOC), and the Gaunt interaction to calculate the electron affinities (EAs) of alkaline earth (AE) metal atoms (Ca, Sr, Ba, and Ra), which are notably small. The coupled-cluster singles and doubles with perturbative triples (CCSD(T)) method is insufficient to accurately calculate the EAs of AE metal atoms. Higher-order excitations proved crucial, with the coupled-cluster singles, doubles, and triples with perturbative quadruples (CCSDT(2)$_Q$) method effectively capturing dynamic electron correlation effects. The contributions of SOC ($\Delta E_{SOS}$) to the EAs calculated using the multireference configuration interaction method with the Davidson correction, including SOC, positively enhance the EAs; however, these contributions are overestimated. The Dirac-Hartree-Fock (DHF)-CCSD(T) method addresses this overestimation and provides reasonable values for $\Delta E_{SO}$ ($\Delta E_{SO-D}$). Employing additional sets of diffuse and core-valence correlation basis sets is critical for accurately calculating the EAs of AE metal atoms. The contributions of the Gaunt interaction ($\Delta E_{Gaunt}$) to the EAs of AE metal atoms are negligible. Notably, the CCSDT(2)$_Q$ with the complete basis set (CBS) limit + $\Delta E_{SO-D}$ + $\Delta E_{Gaunt}$ produced EA values for Ca, Sr, and Ba that closely align with experimental data and achieved accuracy exceeding the chemical accuracy. Based on our findings, the accurately proposed EA for Ra is 9.88 kJ/mol.

# Multireference Configuration Interaction including Spin-Orbit Coupling Study of Potential Energy Curves of gold monotelluride (AuTe) and Energy Levels of Te atom

**Jeongmin Park, Eunji Park, and Joonghan Kim***

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There has been very little theoretical study concerning gold monotelluride (AuTe). We performed state-of-the-art ab initio calculations of the full potential energy curves (PECs) of the various Ω states of AuTe using multireference configuration interaction with the Davidson correction, incorporating spin-orbit coupling (SOC). The various spectroscopic constants of the Ω states of AuTe were also calculated. Additionally, we performed two-component spin-orbit density functional theory (SODFT) calculations to clarify the SO effect on the bond length of AuTe. The first excited state of the Te atom is $^3P_0$, unlike other chalcogen atoms such as O, S, and Se, whose first excited state is $^3P_1$. We elucidated the origin (second-order SOC) of the Te atom that violates Hund's rule. This study is the first to systematically calculate the full PECs and the molecular properties of the ground and excited states of AuTe.



P-35

# Universal Scaling Behavior of Interfacial Thickness in Polymeric Globules

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In this study, we investigate the universal scaling behavior of the interfacial thickness of polymeric globules using parallel tempering molecular dynamics (PTMD) simulations. We model a single polymer as a sequence of Lennard-Jones beads connected by a bonding potential. As the temperature decreases, the polymer adopts a globular and compact conformation due to the increasing influence of attractive interactions between monomers. We find that while conventional theoretical approaches, which assume a sharp interface of globules, effectively describe the temperature dependent size variation of the polymers upon formation of globules, they fail to capture the core density of the globules. This failure is attributed to a substantial interfacial thickness relative to the globule size, suggesting the existence of polymers in an intermediate regime before reaching fully collapsed states. Notably, the observed interfacial thickness displays universal scaling behaviors predicted by previous field-theoretical approaches, affirming the existence of a distinct intermediate globules.

# Uncertainty Quantification of Bayesian Deep Learning ab initio Potential

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Deep learning tools have recently shown outstanding performance in various tasks and attracted significant attention. However, quantifying the prediction uncertainty of these tools, especially for tasks like regression and classification, remains challenging and not fully resolved. In contrast, Bayesian models provide a mathematical framework for handling the current uncertainty logically by learning distributions over weights. However, Bayesian models require substantial modifications to the learning process and incur higher computational costs compared to deep learning models. To address this issue, our goal is to build a transferable Bayesian Deep Learning ab initio Potential for various materials through Bayesian implementation. This aims to combine the advantages of existing deep learning and Bayesian models to effectively handle prediction uncertainty, promising more stable and reliable results. Through this approach, we aim to compare performance in various tasks, including popular alternatives, sample outlier detection, and active learning. Our machine learning potential is expected to effectively handle prediction uncertainty by integrating the strengths of both existing deep learning and Bayesian models, thereby providing more stable and trustworthy results.

# P-37

# Machine Learning-Aided Approach for Charge Transport Dynamics in Organic Semiconductors

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Organic semiconductors possess unique mechanical properties and low-cost processing compared to their inorganic counterparts, making them promising for developing flexible displays, RFID tags and solar cells. Current limitations in our understanding of the fundamental processes behind organic semiconductors hinder the design of next-generation devices with truly high performance. The charge transport in organic semiconductors, which is a critical process in optoelectronic devices, continues to be a subject of active investigation. The complexity arises from the intricate interplay between electrons and nuclei, which governs the dynamics of charge carriers and defies a complete explanation. Nonadiabatic molecular dynamics approaches offer the capability to examine the coupled electron-nuclear dynamics in detail. However, their practical application requires significant advancements in computational efficiency. The immense number of variables including electronic and nuclear degrees of freedom have to be incorporated into the model at every simulation step, making conventional approaches impractical. Existing methods often rely on approximations to improve efficiency, but these can sacrifice accuracy. Our approach addresses this by utilizing machine learning techniques alongside Ehrenfest mean-field dynamics. This combined method, termed Machine Learning-aided Ehrenfest Mean Field (ML-EMF), aims to achieve a balance between accuracy and efficiency. In the presentation, we will present the methodologies and the technical details behind our implementations. We will also unveil some of our preliminary results that demonstrate the capability of the ML-EMF method to capture the charge transport dynamics across different charge transfer regions, formulating a unified approach to describe the complex dynamical processes during charge transportation.

# DFT study of conformers of Haloacetic Acid using Energy Decomposition Analysis

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We employed density functional theory (DFT) calculations to investigate the conformational properties of haloacetic acids (HAAs, $XCH_2COOH$, X=F, Cl, Br, and I), acetic acid derivatives with a hydrogen atom substituted by a halogen atom. The conformers were generated by varying the dihedral angle (∠X-C-C=O, X= F, Cl, Br, and I), and the effects of different halogen substituents (fluorine to iodine) on molecular structure and relative energies were analyzed. The optimal DFT functional (CAM-B3LYP-D3(BJ)) was determined by comparing coupled-cluster singles and doubles with perturbative triples (CCSD(T)) results. Potential energy surfaces (PESs) were then calculated with CAM-B3LYP-D3(BJ) as a function of the HAA dihedral angle. Significant differences in calculated PESs were observed between halogen substituents (see Fig. 1). Energy decomposition analysis (EDA) of HAAs was used to elucidate the origins of these PES variations.

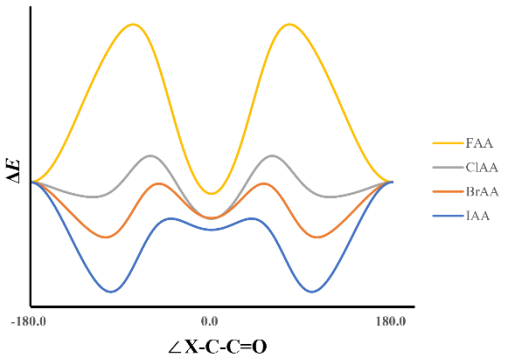



Fig.1: Potential energy surfaces with respect to dihedral angle (∠X-C-C=O, X=F, Cl, Br, and I) of haloacetic acids.

# Application of HF-DFT to the dipole moments of linear molecules

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Understanding and forecasting the physical, chemical, and biological behavior of substances depend extensively on the dipole moments of molecules. In molecular dynamic simulations, dipole moments are also employed to represent long-range electrostatics. The accuracy of the electronic structure calculations is important because the dipole moments can be obtained theoretically through numerical derivatives of energy to the electric field. [1] Because it makes it possible for scientists to accurately and computationally analyze molecular systems and predict their properties, density functional theory, or DFT, has contributed to significant improvements in the field of quantum chemistry.[2] DFT with Hartree-Fock density (HF-DFT) can be a useful way to obtain better results in energies and energy differences of different chemical reactions, but prior research has shown that DFT can be impacted by density-driven errors. The HF density differs significantly from the self-consistent density of systems with large DFT errors not only in terms of energy but also in terms of the dipole moment. We investigate the HF-DFT error for every lung in the Jacobs ladder. When utilizing HF density rather than self-consistent density, a standard procedure has been established to assess the sensitivity of the dipole moment. It is also discussed why dipole moment curves corresponding to non-equilibrium states make HF-DFT physically more valid.

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# P-40

# Exploring Direct Electrochemical Fischer-Tropsch Synthesis of $C_1$-$C_7$ Hydrocarbons via perimeter engineering of Au-$SrTiO_3$ catalyst

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Traditionally, Fischer-Tropsch (FT) synthesis is performed using thermal catalyst and syngas (CO and $H_2$) under high-pressure and high-temperature conditions to produce hydrocarbons. However, this study introduces an approach that relies on the electrochemical (EC) FT synthesis under ambient conditions. A series of $C_nH_{2n+2}$, $C_nH_{2n}$ hydrocarbons (n=1-7) was successfully produced over Au nanoparticle-loaded strontium titanate ($SrTiO_3$) nanostructures grown on rutile ($TiO_2$) supported on Ti. Theoretically, to identify the optimal geometry of supported Au nanoparticles on the perovskite $SrTiO_3$ system and its catalytic active sites, we use a global optimization method that leverages an on-the-fly surrogate Gaussian process regression model and an evolutionary algorithm. This method allows for an effective exploration of the complex energy landscape, identifying low-energy structures. The robust combination of experimental and computational findings reveals that optimum conditions and mechanisms for producing surface hydrogenation and C-C coupling polymerization, initiated by surface *CO and *H, are achieved by controlling the undercoordinated Au at the perimeter sites of supported Au nanoparticles. This EC-FT process opens a promising avenue for the direct conversion of $CO_2$ and $H_2O$ into value-added long-chain hydrocarbons.

# Investigation of Carbene Formation in Ionic Media with Physics-Based, Neural Network Force Fields

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*N*-heterocyclic carbenes (NHCs) rank among the most key catalysts in organic chemistry. There has been recent experimental and theoretical work debating the extent of carbene formation in room temperature ionic liquids (RTILs) at 300 K. The presence of highly reactive carbene species in these conditions can lead toward highly useful applications of RTILs as both a reagent and a solvent. To investigate this question, we run reactive molecular dynamics simulations based on the empirical valence bond (EVB) approach. Our reactive force field combines neural networks with physics-based terms to describe the reacting species within a solution-phase environment. By construction, the neural network terms are restricted to be local and short-range, while long-range interactions are "physics-based" and parameterized based on intermolecular perturbation theory. The neural networks thus allow for modeling of the short-range quantum mechanical degrees of freedom within the reacting complex while maintaining high-accuracy, computationally efficient long-range interactions with the analytic physics-based terms. We use umbrella sampling to construct free energy profiles of the reacting complex in the gas-phase, the bulk IL and at the liquid-vapor interface. We find that the neutral NHC species is destabilized within the liquid phase compared to the gas phase due to the large ion solvation energies. Interestingly, we observe a slight enhancement of the NHC calculated concentration at the interface due to solvophobic interactions.

**Conference funding provided by Dr. Chao-Ping Hsu*

P-42

# Density-based charge partitioning scheme for deep learning applications

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The complications associated with charge partitioning procedures necessitate a new approach to charge analysis, with the aim of obtaining insightful information about the atoms-in-molecules for deep learning applications. From atom-centered, data-driven models like SA-GPR and A2MD to grid-based and message-passing neural network methods, various techniques are being developed to provide reliable and computationally efficient electron density predictions. Building on top of the recent progress in electron density learning, we present a charge density allocation method using the electron density gradient vector field in the molecular plane and promolecular density, which are two fundamental concept in Bader and Hirshfeld partitioning schemes, respectively. We argue that the described formalism can be used to estimate charge transfer values driven by electronegativity differences among atoms-in-a-molecule.

**P-43**

# Quantum-classical hybrid machine learning potential

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The use of quantum algorithms for computationally demanding simulations of large systems has not been extensively explored. Achieving a quantum advantage over existing powerful classical algorithms is currently impractical, so we aim for quantum utility through hybrid quantum-classical algorithms. In this framework, the classical computer handles the main calculations, while a quantum computer deals with specific tasks that need quantum algorithms. In this study, we compared classical neural networks with hybrid quantum-classical neural networks to predict density functional theory (DFT) results for liquid silicon at 3000 K, a challenging scenario for force fields. The classical neural network utilizes the MACE algorithm, while the hybrid quantum-classical neural network incorporated variational quantum circuits alongside the classical components. Using NVT molecular dynamics simulations of liquid silicon at 3000 K, we will discuss the potential of quantum utility in quantum-classical hybrid machine learning.

# Phase Space Nonadiabatic Dynamics with Nonadiabatic Field

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Nonadiabatic dynamics plays a crucial role in the investigation of various significant photochemical processes in chemistry, biology and material science. We present two recent advances in the development of trajectory-based nonadiabatic dynamics methods. One significant development is the establishment of the generalized coordinate-momentum phase space representation for molecular systems. This formalism describes both nuclear and electronic degrees of freedom (DOFs) using continuous coordinates and momenta. The normalization of electronic phase space results in a smooth manifold, which is diffeomorphic to a submanifold of the U(*F*) group. The other advancement is the development of nonadiabatic field (NaF) dynamics. This approach decomposes the force acting on nuclei into two components: the adiabatic force originating from a single electronic state, and the nonadiabatic force arising from the nonadiabatic coupling field. NaF dynamics integrates the benefits of both Born-Oppenheimer dynamics and mean-field dynamics. By implementing NaF dynamics in the generalized coordinate-momentum phase space representation, the resulting novel method demonstrates superior performance compared to conventional methods in numerical simulations of various model systems, including condensed phase dissipative systems, cavity quantum electrodynamics models, gas-phase scattering models, and molecular conical intersection models.

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**P-45**

# Non-negligible outer-shell reorganization energy for charge transfer in nonpolar systems

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Many charge-transporting molecular systems work as ordered or disordered arrays of solid state materials composed of nonpolar (or weakly polar) molecules. Due to low dielectric constants for nonpolar systems, it is common to ignore the effects of outer-shell reorganization energy ($\lambda_{out}$ ). However, ignoring $\lambda_{out}$ has not been properly supported and it can severely impact predictions and insights derived. Here, we estimate $\lambda_{out}$ by two means: from experimental ultraviolet photoelectron spectra, in which the vibronic progression in these spectra can be fitted with the width of the peaks determining $\lambda_{out}$, and from molecular dynamic (MD) simulation of nonpolar molecules, in which disorder or fluctuation statistics for the energy of a charged molecule are calculated. An upper bound for $\lambda_{out}$ was obtained as 505 and 549 meV for crystalline anthracene (140K) and pentacene (50K), respectively, by fitting of experimental data, and 212 and 170 meV, respectively, from MD simulations. These values are comparable to the inner-sphere reorganization energy ($\lambda_{in}$) arising from intramolecular vibration. With corresponding spectral density functions calculated, we found that $\lambda_{out}$ is dominated by low-frequency dynamics, indicating that constrained translational and rotational motions of surrounding molecules are important in accommodating the charge. Moreover, crystalline systems exhibit super-Ohmic spectral density, whereas amorphous systems are sub-Ohmic.

# Aharonov-Bohm Effect at Finite Temperature

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The Aharonov-Bohm effect, initially proposed by Y. Aharonov and D.J. Bohm in 1959 [1], is a fundamental quantum phenomenon where the trajectory of an electron is influenced by the vector potential induced by a magnetic field, independent of the presence of a substantial magnetic field. Over the years, this effect has been extensively studied in conjunction with advanced physical concepts like the Berry phase, leading to its application in various fields, underpinning an understanding of topological properties. Experimental verification of this effect was achieved by A. Tonomura *et al.* in 1986 [2], providing pivotal evidence of its existence. Our study explores novel aspects of the thermal characteristics associated with the Aharonov-Bohm effect. Despite limited literature directly addressing its thermal implications, we thoroughly investigate its thermal influence using density operators and quantum master equations. Our analysis not only encompasses equilibrium phenomena but also extends to non-equilibrium dynamics induced by heat sources. To comprehensively explore these thermal effects, we leverage both the conventional Caldeira-Leggett model [3] and the RISB model proposed by Y. Iwamoto and Y. Tanimura in 2018 [4].

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**P-47**

# Spatio-Temporal Characterization of Water Diffusion Anomalies in Saline Solutions Using Machine Learning Force Field

**Ji Woong Yu**

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Force fields are essential for simulating chemical systems by capturing atomic interactions. However, many force fields struggle to accurately describe the behavior of water in salt solutions, failing to reproduce the experimentally observed effects of kosmotropic and chaotropic salts on water dynamics, known as the Hofmeister series. This study presents a comparative analysis of various force fields, including SPC/Fw+JC, AMOEBA, MB-Pol, AIMD (BLYP-D3), and a novel machine learning force field (MLFF), Deep Potential Molecular Dynamics (DPMD), in their ability to capture the effects of salts on water dynamics.

The four-point susceptibility of water in salt solutions, a measure of spatio-temporal correlation, is used to assess the effectiveness of each force field. The length and timescale associated with the four-point susceptibility are packed into an order parameter correlation-scaled diffusivity, which is proportional to diffusivity. This proportionality supports the idea that proper capture of correlated water dynamics is key to understanding the enhancement or retardation of water dynamics in salt solutions.

Among the models considered, DPMD is the only force field that accurately captures the diffusivity trend, except for AIMD. However, AIMD cannot be scaled to a size and timescale with which four-point susceptibility can be calculated, making DPMD even more useful in the computational study of salt solutions. The results of this study highlight the significant potential of machine learning force fields for more accurate simulations of complex aqueous systems.

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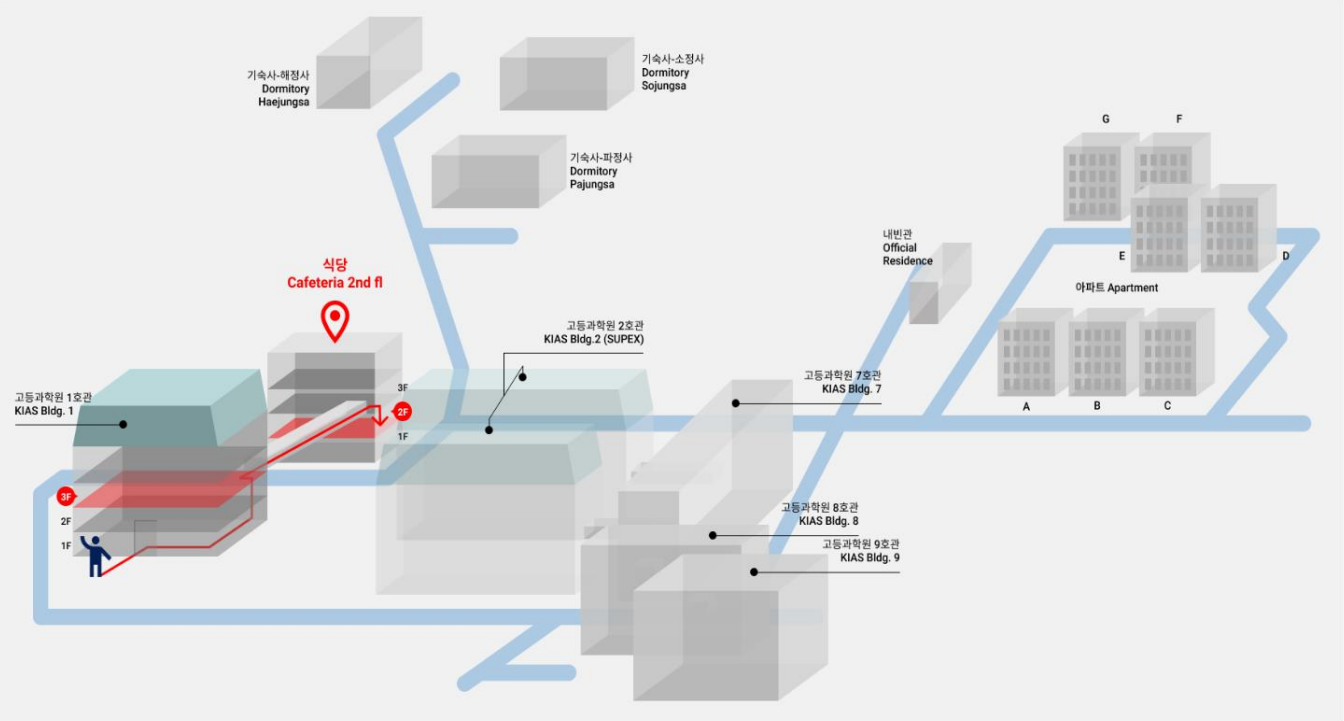
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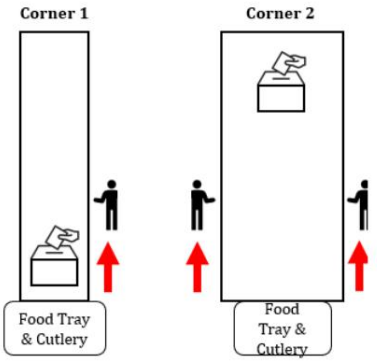
### Bldg.1 to Cafeteria

1. Go downstairs to the 3rd floor of the main building(Bldg.1).
2. Use the passageway that connects the buildings. Just go straight forward and if you see Woori-Bank, it means that you arrived at the student union building 3rd floor correctly.
3. Go downstairs one more time. The cafeteria is one the 2nd floor of the student union building.

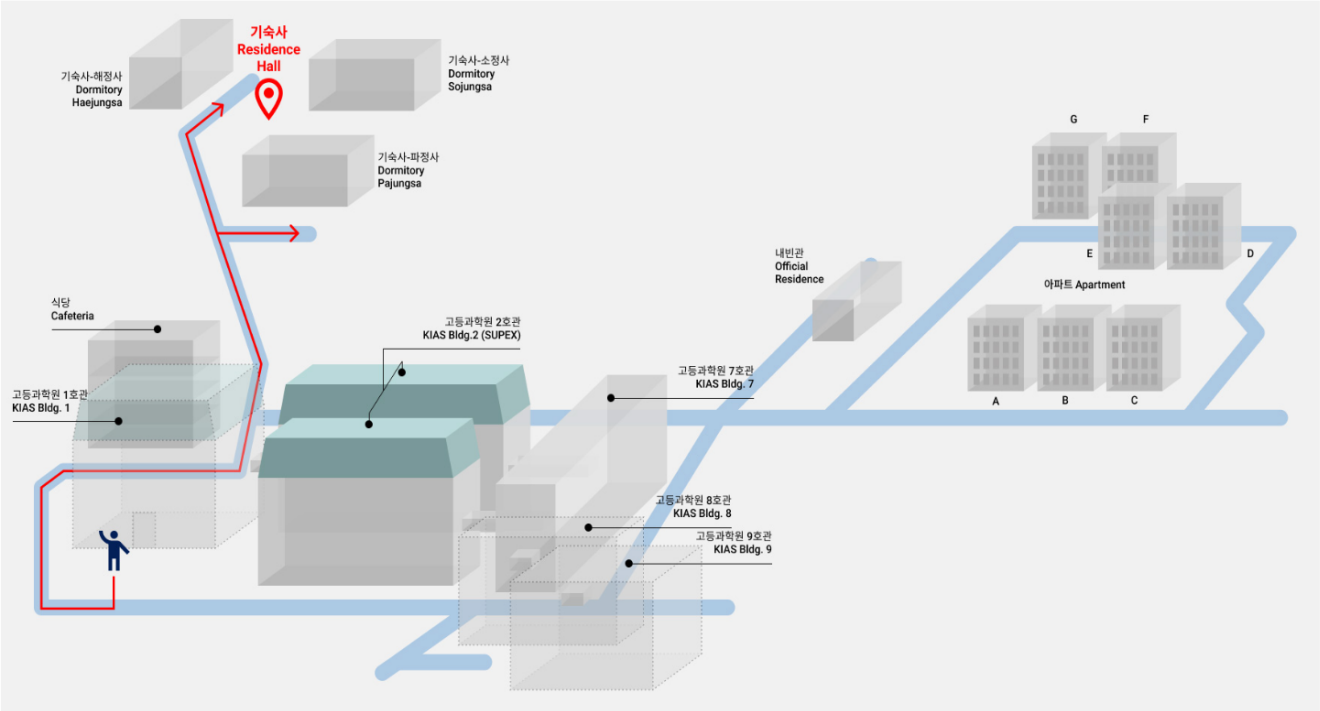



### Lunch Coupon Usage

- You can pick up lunch coupons at the reception desk in front of the 1503 seminar room.
- These coupons can be used at the KIAS cafeteria only during lunch time (12:00~13:00).
- Today's menu is displayed outside the cafeteria and each corner has different menu. Please choose one.
- Please put the lunch coupon inside the transparent ticket box. Box location is different by Corners. (Please refer to the image)



### Bldg.1 to Residence Hall




### Transportation

Bus – 201, 273

- Get off at 'KAIST /Hong-neung Elementary School'.

Metro – line no.1

- Get off at 'Cheongnyangni' or 'Hoegi' Station.

From Hoegi Station

1. From exit No. 1, turn left and follow the sidewalk on the right until you reach the intersection and crosswalk.
2. Cross the street and turn right.
3. Go straight until you see the bus stop.
4. Take No.273 and get off at 'KAIST /Hong-neung Elementary School'.

From Cheongnyangni Station

1. When you get out through exit No. 2, ignore the bus stop you see right away and follow the way without making turns until you see another bus stop.
2. Take No. 201 and get off at 'Hong-neung Elementary School' bus stop.
3. You will see KIAS(KAIST campus) across the street.