

시스템화학 글로벌 선도연구센터

1 차년도 동계 학술대회

일시: 2025 년 2 월 25 일 (화) 13:00-21:00, 26 일 (수) 09:00-20:00

장소: 중앙대학교 310 관 B603 호 (oral session)

중앙대학교 102 관 11 층 세미나실 (poster session)



주최: 시스템 화학 글로벌 선도연구센터 (GCSC)

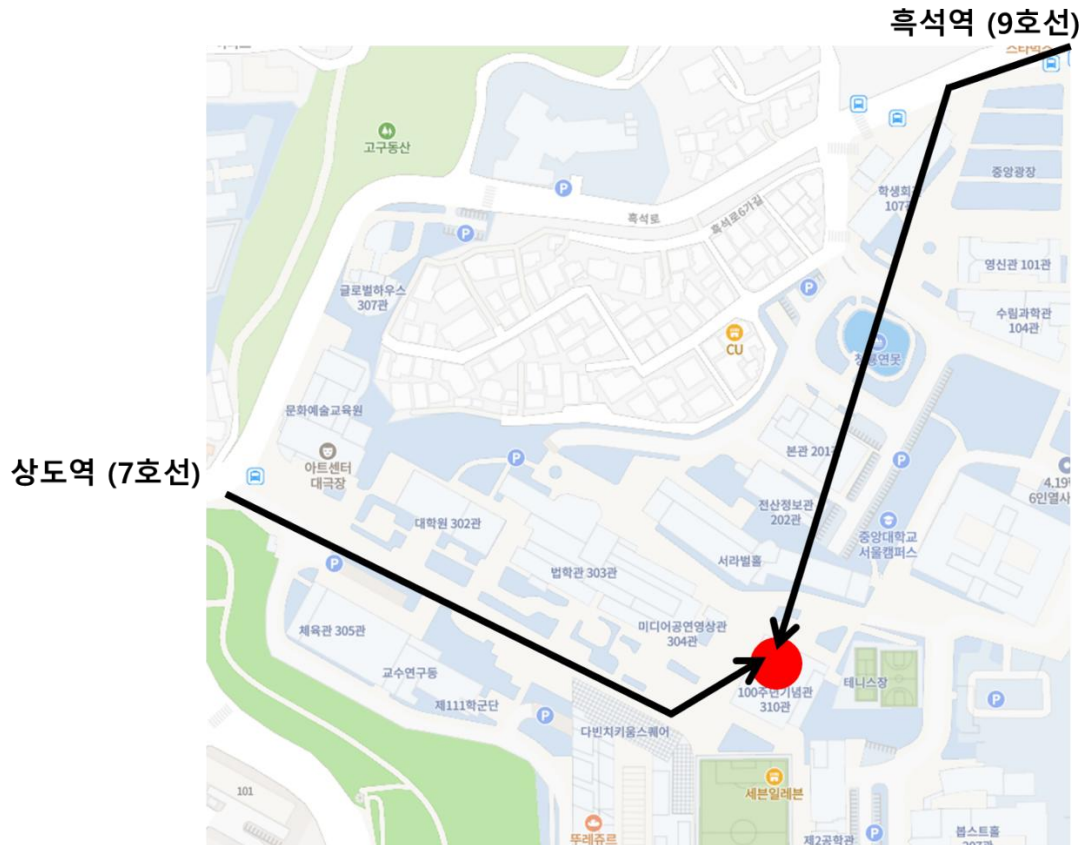
후원: 중앙대 화학과 BK21 (생물리광화학창의인재양성팀)

중앙대 신기능이미징연구소

학술대회 장소 안내

장소: 서울시 동작구 흑석로84 중앙대학교 310관 B6 603호

오시는 길



지하철

9호선 흑석역(중앙대 입구역): 3,4번 출구에서 도보 10분

일반버스

지선버스 5511(서울대->중앙대), 5517(서울대->중앙대), 5524(신림8동->중대입구):

중앙대정문 하차

간선버스 151(우이동->중앙대): 중앙대병원 하차

360(송파->흑석역): 흑석역 하차

프로그램

2 월 25 일 (화)

사회: 심상희 교수 (고려대)

13:00~13:30	등록
13:30~13:40	개회사: 대한화학회 53대 회장 신석민 교수 (서울대) 축사
13:40~13:50	센터장 환영사 및 주요 업무보고
Session 1 좌장: 장락우 교수 (서울시립대)	
14:00~14:30	장준경 교수 (부산대학교 나노에너지공학과) Molecular Structure of Interfacial Water
14:30~15:00	임미희 교수 (KAIST) Chemical (Bioinorganic) Strategies to Study Multiple Facets in Dementia
15:00~15:10	Coffee break
Session 2 좌장: 정연준 교수 (서울대)	
15:10~15:40	이강택 교수 (광주과기원)
15:40~16:10	이남기 교수 (서울대)
16:10~16:20	Coffee break
Session 3 좌장: 김지현 교수 (중앙대)	
16:20~16:50	이정욱 교수 (포항공대)
16:50~17:20	장성호 교수 (인천대)
	Banquet

2월 26일 (수)

9:00~9:10	등록
Session 4 좌장: 최정모 교수 (부산대)	
9:10~9:40	성주영 교수 (대구과기원)
9:40~10:10	고두현 교수 (성균관대) Suppressing Phase Separation in Organic Bulk-Heterojunctions through a Multicomponent System
10:10~10:20	Coffee break
Session 5 좌장: 고혜란 교수 (중앙대)	
10:20~10:50	이상학 교수 (부산대) Chemical framework for understanding Neurodegenerative Diseases
10:50~11:20	김두리 교수 (한양대)
11:20~11:30	Coffee break
Session 6 좌장: 조해성 교수 (중앙대)	
11:30~12:00	이원희 교수 (KAIST)
12:00~12:30	성재영 교수 (중앙대)
12:30~14:00	점심식사 (황토정)
Poster session	
14:00~15:50	포스터 발표
15:50~16:00	우수 포스터 수상
16:00~17:50	시스템화학 연구센터 연구모임
1차년도 성과 점검 및 2차년도 연구 추진 회의	
18:00~20:00	저녁식사 및 시스템화학 연구센터 운영회의

Oral Session

Abstract

(Session X-X)

Title of presentation

Name^{1*}

Affiliation

You can write the abstract here. If you have any papers you would like to cite, please include citations like "[1]" or "[2]" in the text and list the references below. [1-2] The abstract should briefly summarize the content of your presentation.

Reference

[1]

[2]

(Session 1-2)

Chemical (Bioinorganic) Strategies to Study Multiple Facets in Dementia

Mi Hee Lim^{*}

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Daejeon 34141, Korea*

Alzheimer's disease (AD), associated with degeneration of neurons and synapses in the brain, leads to motor impairment and eventual fatality. Neurodegeneration could be related to various interconnected features, including (i) plaque formation from amyloid- β (A β) peptide fragments, (ii) metal ion dyshomeostasis and miscompartmentalization, as well as (iii) inflammation and increased oxidative stress due to overproduction of reactive oxygen species (ROS). The inter-relations between some of these pathological factors have been investigated. Metals are found entangled in the A β plaque and likely contribute to A β neurotoxicity and oxidative stress. ROS have been shown to increase the rate of A β plaque formation. Our understanding of the correlation between these elements and AD neuropathogenesis has been very limited, however. There is currently no cure for AD; therapies are focused on symptomatic relief targeting the decrease in the levels of acetylcholine, only one of the multiple factors causing the disease [1-3]. To find a cure for AD, we require a better understanding of the relationship between various causative factors of this devastating disease. Towards this goal, we have been developing suitable chemical tools capable of targeting and regulating multiple underlying factors or identifying the pathogenic networks composed of their direct interactions and reactivities [4-13].

References

- [1] *Chem. Rev.* **2019**, *119*, 1221.
- [2] *Acc. Chem. Res.* **2014**, *47*, 2475; *Acc. Chem. Res.* **2021**, *54*, 3930.
- [3] *Coord. Chem. Rev.* **2023**, *478*, 214978.
- [4] *Proc. Natl. Acad. Sci. USA* **2010**, *107*, 21990.
- [5] *Chem. Sci.* **2015**, *6*, 1879.
- [6] *J. Am. Chem. Soc.* **2014**, *136*, 299.
- [7] *J. Am. Chem. Soc.* **2015**, *137*, 14785.
- [8] *Nat. Commun.* **2016**, *7*, 13115.
- [9] *Proc. Natl. Acad. Sci. USA* **2020**, *117*, 5160.
- [10] *J. Am. Chem. Soc.* **2020**, *142*, 8183.
- [11] *Nat. Chem.* **2022**, *14*, 1021.
- [12] *Adv. Sci.* **2024**, *11*, 2307182.
- [13] *Nat. Chem. Biol.* **2024**, *In Revision*.

(Session 4-2)

Suppressing Phase Separation in Organic Bulk-Heterojunctions through a Multicomponent System

Doo-Hyun Ko^{1*}

¹ Department of Chemistry, Sungkyunkwan University, Suwon 16419 Korea

The unique properties of organic photovoltaics (OPVs) hold great promise for emerging applications such as the Internet of Things. The long-term stability of OPVs is a critical factor for their practical use in commercial fields. In addition to solar light, OPVs should be designed to operate under versatile irradiation circumstances, as they need to provide electric power for 24 hours. In this study, we report on multi-component OPVs that simultaneously improve efficiency and extend lifetimes. The multi-component blends exhibit a broadened spectral response and improved charge transport process with suppressed recombination, resulting in high output powers capable of powering low-power electronic devices. Furthermore, the aggregation of meta-stable molecules was notably reduced in the multi-component blend. The combination of high efficiency, improved device lifetimes, and the use of multi-component blends offers promise for commercially viable OPVs in various applications.

(Session 5-1)

Chemical framework for understanding Neurodegenerative Diseases

Jinmin Lee and Sang Hak Lee^{1*}

¹ Department of Chemistry, Pusan National University, Busan 46241, Korea

The study of non-bonding interactions has transcended the exclusive domain of physical chemists employing spectroscopy and computer simulations. With the advent of molecular biology, non-bonding interactions have emerged as pivotal factors in comprehending the structures and functionalities of biomolecules, including DNA and proteins. Among these non-bonding interactions, ionic interactions stand out as the most robust forces mediating interactions between anionic and cationic molecules. When scrutinizing the intracellular milieu, non-bonding interactions, particularly those of the ionic nature, wield significant influence over protein-protein and DNA-protein interactions. Consequently, we hypothesized that protein aggregation or phase separation, known contributors to neurodegenerative diseases such as Alzheimer's, Parkinson's, and Lou Gehrig's diseases, may also be governed by these ionic interactions. Given the highly charged nature of disease-related proteins, a substantial charge disparity exists, making self-aggregation in the absence of cofactors a formidable challenge. Our research has yielded a compelling insight: small (negatively or positively) charged biomolecules play a pivotal role in facilitating the formation of protein condensates through ionic interactions within cellular environments.

Poster Session

Abstract

(Poster XX)

Title of presentation

Name^{1*}

Affiliation

You can write the abstract here. If you have any papers you would like to cite, please include citations like "[1]" or "[2]" in the text and list the references below. [1-2] The abstract should briefly summarize the content of your presentation.

Reference

[1]

[2]

(Poster 1)

Machine Learning to Predict the Photovoltaic Parameters of Organic Bulkheterojunction

Chihyung Lee, Hyeonjin Choi, Doo-Hyun Ko^{1*}

¹ *Department of Chemistry, Sungkyunkwan University, Suwon 16419 Korea*

Machine learning (ML) to predicting power conversion efficiency (PCE) of organic photovoltaics (OPVs) have attracted due to reduction of the labor-intensive trial-and-error. Although the previous OPV-ML models achieve high predictive PCE accuracy, they still face challenges due to their reliance on chemical properties of materials as input data.[1-2] The previous OPV-ML models are limited in their applicability as they require the accurate determination of material properties through experiments before screening, which hinders the practical use of OPV-ML models. Here, to streamline the laborious process, we introduce the unique structural-feature descriptor that expresses desired structures as low-dimensional matrices. This descriptor simplifies the expression of structures by indexing functional group units as positive integers and combining the indices to form a concise matrix. This concise expression enables the models to easily track and prioritize functional groups that significantly contribute to PCEs. The proposed model achieves a high Pearson's coefficient of 0.86 between real and predictive PCEs, despite using only the descriptor of molecular structures without any additional properties. Our novel descriptor provides valuable guideline for designing new conjugated materials and promises a effective screening tool for the blend candidates.

(Poster 2)

Kinetic Analysis of p53 Regulation in Cancer Cells

Sangmin Ji and Hye Ran Koh*

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The tumor suppressor protein p53 plays a pivotal role in maintaining genomic integrity by regulating the transcription of genes involved in DNA repair, cell cycle arrest, and apoptosis. *TP53*, a gene encoding p53, is the most frequently mutated gene in human cancers, highlighting its critical role in tumor suppression. Consequently, targeting the p53 pathway represents a promising strategy for anticancer drug development. One key regulator of p53 is MDM2, a p53-induced gene whose protein product facilitates p53 degradation through ubiquitination, thereby maintaining p53 at low levels. Here, we investigated the regulation of p53 expression in A549 cells, a cancer cell line with low p53 levels due to MDM2 overexpression. Using single-molecule fluorescence *in situ* hybridization and immunofluorescence, we examined the effects of Nutlin-3a, an MDM2 inhibitor, on p53 dynamics. Upon Nutlin-3a treatment, we observed a significant increase in p53 expression and a corresponding reduction in cell viability. Furthermore, we quantitatively analyzed p53 expression at both the mRNA and protein levels over time following MDM2 inhibition. This kinetic analysis provides valuable insight into the temporal dynamics of p53 activation in response to MDM2 inhibition, which may contribute to optimizing therapeutic strategies targeting the p53 pathway for cancer treatment.

(Poster 3)

Thickness-Dependent Relaxation of Near-IR Excitons in 2D CrCl₃ Crystals

Hyesun Kim and Sunmin Ryu*

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Two-dimensional (2D) chromium(III) chloride (CrCl₃) is promising for optoelectronic devices and magnetic sensors because of its intrinsic magnetism in the monolayer limit and strong visible absorption of its bulk form.[1] In this work, we studied the electronic structure and excitonic behaviors of few-layer to bulk CrCl₃ using absorption, photoluminescence (PL) spectroscopy and time-correlated single-photon counting (TCSPC). There was no significant spectral change in the absorption and PL signals for 2D and 3D crystals, which may originate from a localized nature of the near-IR excitons. Surprisingly, however, the PL lifetime showed a drastic reduction from 4.5 μ s to 0.7 ns with decreasing thickness from bulk to 1.4 nm. Control experiments with UV-generated ozone and crystalline hexagonal BN substrates indicated that structural defects are responsible for the accelerated relaxation in 2D forms. TCSPC measurements with control on temperature and wavelength suggested that the PL of CrCl₃ has more than one origin, with vacancies and oxidized surfaces possibly contributing to these effects. Preliminary PL experiments using a gas cell suggest that the reaction with water may be partially reversible. This study will contribute to the mechanistic understanding of the excitonic relaxation and device application of the 2D magnetic semiconductor.

Reference

- [1] Michael A. McGuire, Genevieve Clark, Santosh KC, W. Michael Chance, Gerald E. Jellison, Jr., Valentino R. Cooper, Xiaodong Xu, and Brian C. Sales, Phys. Rev. Materials 1, 014001 (2017).

(Poster 4)

Charge-Transfer & Energy-Transfer at Two-Dimensional PTCDA on TMD Heterocrystals

Eunbeen Jeon, and Sunmin Ryu*

*Department of Chemistry, Pohang University of Science and Technology (POSTECH),
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Two-dimensional (2D) layered materials, transition metal dichalcogenides (TMDs) have been studied extensively due to their high charge mobility and excellent optical transparency. Organic semiconductors of the π -conjugated molecule series have the advantage of strong light sensitivity and high absorption in the visible light range. Recently, considerable efforts have been devoted to engineering hybrid organic-inorganic heterostructures. However, challenges persist in achieving high crystallinity at the atomically thin limit and elucidating the interfacial charge transfer mechanisms with precision. In this study, we successfully synthesized highly crystalline PTCDA-TMD heterostructures with well-defined thickness modulation at the few-layer level via a physical vapor deposition (PVD) system. The epitaxial alignment and crystallographic orientation between the organic and inorganic constituents were systematically investigated through electron diffraction and polarization-resolved spectroscopy. Additionally, the layer-dependent optical properties of PTCDA were quantitatively analyzed using absorption spectroscopy, while photoluminescence measurements across varying inorganic substrates provided insights into the band structure evolution and charge transfer dynamics within the heterojunction. This study is expected to contribute to the development of low-dimensional organic-inorganic heterojunction semiconductors and may be utilized in future optoelectronic device applications.

(Poster 5)

Excitonic Behaviors of 2D Tetracene Crystals Using Absorption and Emission Spectroscopies

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Investigating the behavior and characteristics of molecular excitons in low-dimensional molecular solids is crucial for advancing our understanding of fundamental chemical principles and photonic applications. However, research in this area remains in its early stages, and a comprehensive theoretical and experimental framework has yet to be fully established. In this study, we report the temperature-dependent excitonic behaviors of mechanically exfoliated two-dimensional Tetracene (Tc) crystals through absorption and photoluminescence spectroscopies. Polarization-resolved measurements reveal that the transition dipole moment of tetracene is oriented along its short molecular axis. Furthermore, we demonstrate that the trap states emerging at low temperatures are intrinsic in nature, as evidenced by their correlation with a phase transition, confirmed through polarization-dependent spectroscopy. We observe that the Davydov splitting energy increases with decreasing temperature, which we attribute to changes in the exciton bandwidth. Our findings provide deeper insight into the excitonic behavior of 2D molecular crystals, significantly advancing the current understanding in photophysical principles.

Reference

- [1] Sang-Hyun Lim, Thomas G. Bjorklund, Frank C. Spano, and Christopher J. Bardeen, *Physical review letters* **2004**, 92 (10), 107402.
- [2] Seonghyun Koo, Ina Park, Kenji Watanabe, Takashi Taniguchi, Ji Hoon Shim, and Sunmin Ryu, *Nano Lett.* **2021**, 21 (15), 6600–6608.
- [3] Dogyeong Kim, Sol Lee, Jiwon Park, Jinho Lee, Hee Cheul Choi, Kwanpyo Kim, Sunmin Ryu, *Nature communications* **2023**, 14 (1), 2736.
- [4] Voigt M, Langner A, Schouwink P, Lupton JM, Mahrt RF, Sokolowski M, *J. Chem. Phys.* **2007**, 127 (11), 114705.
- [5] Jonathan J. Burdett, David Gosztola, Christopher J. Bardeen, *J. Chem. Phys.* **2011**, 135 (21), 214508.

(Poster 6)

Second-Order Susceptibility Change in 2D Hexagonal BN by Neighboring Excitons

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Due to its high sensitivity in many two-dimensional (2D) materials, second-harmonic generation (SHG) spectroscopy has been widely used to understand how their nonlinear susceptibility is affected by energy and charge transfer from neighboring materials.[1] In this study, we explored the possibility that excitons in proximity modulate the SHG signals of 2D dielectrics that cannot accept the excitonic energy or charge. 2D heterostructures of hexagonal BN and WS₂ were prepared by conventional mechanical exfoliation and dry transfer. To distinguish the SHG signals of hexagonal BN modulated by the proximity effect from those of WS₂, specific layer configurations were selected and technical methodologies were employed. The SHG enhancement by the presence of the WS₂ layer determined over a wide SH energy (2.35 ~ 3.18 eV) exhibited intriguing spectral structures, which may relate to the WS₂ excitons. The excitonic proximity effects in SHG will serve as a novel route for inter-material interactions, potentially leading to applications in optoelectronic devices such as next-generation semiconductors integrated with TMDs.

Reference

[1] W.Kim, et al. *ACS Nano* 17, 20 (2023): 20580-20588

(Poster 7)

Quantitative understanding of bacterial stress responses using new chemical dynamics model for bacterial growth and persistence

Jae Hyuk Won, Ji-Hyun Kim* and Jaeyoung Sung*

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Microorganisms endure harsh environments by dynamically adjusting their transcriptional programs, often through competition between the housekeeping sigma factor RpoD and the alternative sigma factors. Under stress, the alternative sigma factor RpoS—a master regulator of stress response genes—accumulates and induces protective responses; however, once stress is removed, RpoS levels decrease and RpoD regains dominance, driving cell recovery and growth. Here, we introduce a new chemical dynamics model that captures this post-stress transition in *Escherichia coli*. Guided by experimental data on the timing of first cell division after stress, our model quantitatively reproduces how *E. coli* populations resume growth. These findings highlight the critical role of sigma factor switching in coordinating bacterial adaptation and persistence, offering a clearer picture of how cells reestablish normal physiology once external pressures subside. This framework may provide valuable insights for developing strategies to control persistent infections and enhance the effectiveness of antimicrobial therapies.

(Poster 8)

Analyzing Fluorescent Protein Expression in Living Cells: A Novel model Integrating Gene expression, Maturation, and Degradation Dynamics in Response to External Signaling

Jinhyung Kim^{1,2}, Seong Jun Park^{2,3}, Ji-Hyun Kim^{1,2} and Jaeyoung Sung^{1,2*}

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Fluorescent proteins are effective tools for quantifying gene expression dynamics in living cells. While it is known that these proteins emit fluorescence upon undergoing maturation processes, the impact of these processes on protein levels measurable by fluorescent proteins remains unclear. Here, we propose a new version of the chemical fluctuation theorem (CFT)¹ that applies to fluorescent proteins expressed in a burst manner and can be used to analyze experimental observables such as the mean and variance of matured protein levels in living cells. We also explore intracellular response dynamics triggered by external stimuli such as transcriptional induction or antibiotic stress. This research provides a reliable and quantitative tool to analyze time-dependent cellular response to various signals.

Reference

- 1 Park, S. J. *et al.* The chemical fluctuation theorem governing gene expression. *Nature communications* **9**, 1-12 (2018).

(Poster 9)

Multiphasic size-dependent growth dynamics of nanoparticle

Ji-Hyun Kim^{a,b,c,†}, Joodeok Kim^{d,e,†}, Byung Hyo Kim^{d,e,f,†}, Sanggeun Song^{g,h,†},
Hoje Chunⁱ, Hyesung Choi^{d,e}, Hyungjin Cho^f, Yongjoon Kim^f, Jae Won Jung^f,
Youngju Sohn^{d,e}, Junhyeok Jeong^{d,e}, Kunwoo Park^{d,e}, Jinho Rhee^{d,e}, Sungho Jeon^j,
Jingyu Kang^{a,b,c,k}, Minho Lee^{a,b,c,k}, Byungchan Hanⁱ, Won Chul Lee^j,
Taeghwan Hyeon^{d,e,*}, Jaeyoung Sung^{a,b,c,k,*}, Jungwon Park^{d,e,l,m,*}

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[†]These authors contributed equally to this work.

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Colloidal nanoparticles are widely studied in science and industry, yet their thermodynamic mechanisms and growth dynamics remain elusive. Here, we investigated hundreds of in-situ growth paths of a nanoparticle group using liquid-phase TEM, uncovering size-dependent multiphasic growth dynamics inconsistent with current theories. Based on these observations, we developed a novel model and theory for growing nanoparticle ensembles, offering a comprehensive, quantitative understanding of time-dependent size averages, fluctuations, and size-dependent growth rates across diverse nanoparticle systems. Our findings indicate significant deviations from the Gibbs-Thomson equation in small nanoparticles, illuminating its role in governing size-dependent growth dynamics.

(Poster 10)

Supersaturation, Nucleation, and Phase Separation of Mesoscopic Systems

Jingyu Kang^{1-3†}, Donghee Kim^{1-3†}, Sanggeun Song^{4,5†}, Jonghwa Han¹⁻³, Ji-Hyun Kim^{1-3*}, and
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Supersaturation, nucleation, and phase separation are ubiquitous phenomena of great interest in both science and industry. However, a unified, quantitative understanding of these phenomena has yet to be achieved for mesoscopic systems. Here, we present a set of general equations that determine the monomer saturation degree, the size distribution and free energy of mesoscopic systems, as well as their phase transition conditions. These equations reveal that, under supersaturation, the largest cluster size (LCS) is an important state-variable; the supersaturation degree decreases with the LCS, approaching unity in the macroscopic limit. We identify the critical supersaturation condition, above which the nuclei undergo the phase transition to form large crystals. Below this critical supersaturation, the nucleus size distribution is either a unimodal function or a monotonically decreasing function of size, depending on system and temperature. We also predict the most probable nucleus size and the direction of spontaneous changes of the LCS. This work will serve as a general theoretical framework for understanding, predicting, and designing nucleation and phase transitions in mesoscopic systems.

(Poster 11)

Metabolism-inspired chemical reaction networks for chemically driven dissipative oligoesterification

Yeonsoo Lim^{1,+}, **Gyunam Park**^{1,2,+}, Hojin An^{1,+}, Jonghwa Han^{1,2}, Joonhyun Bae³, Ji-Hyun Kim^{1,2}, Yan Lee^{*4}, Kyungtae Kang^{*3}, Jaeyoung Sung^{*1,2}, and Sunbum Kwon^{*1}

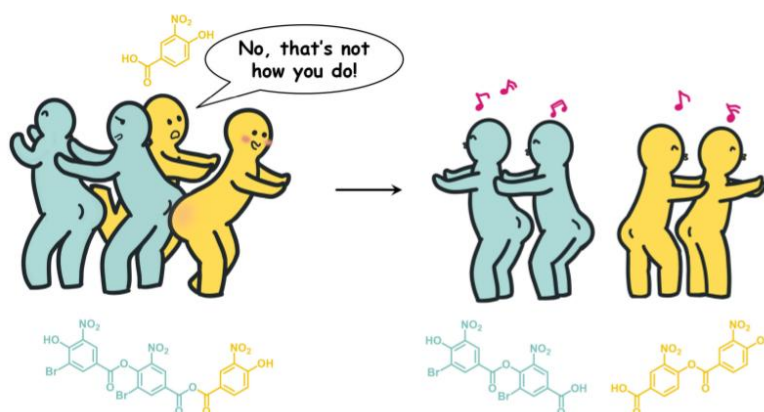
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⁴ Department of Chemistry, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea

Metabolism is a complex network of chemical reactions in which transient biomolecules are continuously produced and degraded. Mimicking this dynamic process in synthetic systems poses a considerable challenge, as it requires designs that enable the exchange of energy and matter among transient molecules. In this study, we explored a chemically driven oligoesterification process operating within a highly intricate reaction network and constructed a dynamic library of transient oligoesters. Our kinetic analysis uncovered an intriguing phenomenon: oligoesters undergo parasitic exchanges, consuming one another to sustain the system's dynamics before reaching thermodynamic equilibrium. This discovery opens new opportunities for designing synthetic systems that replicate the complexity and self-sustaining behavior of metabolic processes.



(Poster 12)

Graph Networks with Transfer Learning Strategy for Multicomponent Property Prediction

Seongmin Yoo, Ji-Hyun Kim* and Jaeyoung Sung*

Department of Chemistry, Chung-Ang University, Seoul

The precise prediction of material property holds substantial industrial and scientific significance, though current deep learning methods have primarily focused on single molecules with simplistic representations that inadequately capture molecular interactions and compositional effects. To address these limitations, we present a comprehensive graph-based deep learning framework that significantly enhances prediction performance in multicomponent systems. Our model implements a three-fold strategy anchored by transfer learning from pure systems to enhance model robustness. The streamlined sequence begins with a pre-trained graph transformer processing molecular information, followed by a gate module governing multiple parallel networks handling diverse property ranges, and concludes with a feed-forward neural network for final predictions. Preliminary results demonstrate significant potential in advancing molecular property prediction through this innovative three-tier architecture. This comprehensive approach, combining sophisticated molecular representations and transfer learning strategies, yields promising improvements in prediction accuracy and computational efficiency, marking a substantial advancement in molecular modeling.

(Poster 15)

Pd Nanoparticles Immobilized on Bipyridine-Functionalized Covalent Triazine Frameworks for Catalytic Nitrobenzene Reduction

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The development of highly efficient and stable catalytic systems for nitroarene reduction is of significant interest in industrial research. In this study, we report the synthesis of palladium (Pd) nanoparticles immobilized on bipyridine-functionalized covalent triazine frameworks (Pd@bpyTN-CTF) as a robust heterogeneous catalyst for the selective hydrogenation of nitrobenzene. The bipyridine moieties within the CTF structure provide strong coordination sites for Pd nanoparticles, leading to uniform dispersion and enhanced catalytic stability. The Pd@bpyTN-CTF catalyst exhibits excellent catalytic performance with high conversion rates and selectivity under mild reaction conditions. Detailed characterization, including TEM, and BET analysis, confirms the well-dispersed Pd nanoparticles and the porous nature of the CTF support. This work highlights the potential of functionalized CTFs as promising platforms for the immobilization of metal nanoparticles in catalytic applications.

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(Poster 16)

Pd-Xantphos catalyzed carbonylative ring closing cyclization of unsaturated alcohol to lactone and its mechanism

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Since the successful debut of Reppe carbonylation, hydroxy-/alkoxy-carbonylation utilizing transition metal catalysis has found diverse applications. Particularly, alkoxy-carbonylation has evolved as an effective method to obtain acids and ester derivatives with high conversion rates and selectivity, contributing to various fields such as plastic and pharmaceutical synthesis. In this experiment, as a part of alkoxy-carbonylation, carbonylative ring closing cyclization of 3-buten-1-ol was conducted using palladium(ii) trifluoroacetate, xantphos, and para-toluenesulfonic acid monohydrate, resulting in the generation of g-valerolactone and d-valerolactone. d-Valerolactone emerged as the major product, and DFT calculations confirmed that this outcome is attributed to the stability of intermediates rather than thermodynamic stability. These results present a novel example of unsaturated alcohol lactonization and contribute to a deeper understanding of the reaction mechanism.

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(Poster 17)

Hybrid Resolution Exchange Molecular Dynamics Simulation Methods for Effective Sampling of Intrinsically Disordered Proteins

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Intrinsically disordered proteins (IDPs) exhibit complex energy landscapes with high energy barriers between states[1], making their molecular dynamics (MD) simulations particularly challenging. Conventional MD methods such as all-atom (AA)[2] and coarse-grained (CG)[3] models utilize various levels of atomic resolutions, each with inherent advantages and limitations. For instance, AA models offer high accuracy but encounter significant energy barriers, while CG models reduce these barriers at the cost of detailed information. To overcome these challenges, we combined both AA and CG models through a Resolution Exchange MD (REMD) framework. This hybrid approach facilitates dynamic transitions between AA and CG resolutions, enabling accurate representation of complex systems. We evaluated this method using a binary mixture system, comparing their mixing behaviors in pure AA simulations versus hybrid REMD simulations.

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(Poster 18)

**Molecular Dynamics Simulation Studies
on the Binding Mechanism of LiPF₆
in Organic Solvents Using Umbrella Sampling**

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This study quantitatively analyzes the binding behavior of lithium hexafluorophosphate (LiPF₆) electrolytes in nonaqueous solvents, a critical factor influencing ion transport and the overall performance of lithium-ion batteries (LIBs). To achieve this, molecular dynamics (MD) simulations combined with the umbrella sampling method were employed to compute the binding free energy of LiPF₆ ion pairs in organic solvents with different dielectric constants (ϵ). In particular, the effects of dielectric properties on ion pairing and dissociation were investigated by comparing dimethyl carbonate (DMC) and propylene carbonate (PC). The results indicate that in low- ϵ solvents like DMC, LiPF₆ ion pairs exhibit strong interactions, leading to stable aggregation structures, which hinder dissociation and potentially reduce ion conductivity. In contrast, ion pairs dissociate more easily in high- ϵ solvents such as PC, facilitating solvation, resulting in a more uniform ion distribution and reduced aggregation.[1-2] Additionally, machine learning potentials (MLP) will be introduced in future studies to incorporate charge polarization effects more accurately. This approach is expected to overcome the limitations of conventional charge scaling methods and enable more reliable ion dynamics simulations.[3]

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(Poster 19)

Chemical Property Prediction Using In-Context Learning in Large Language Models

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Recent advances in AI, particularly transformer-based large language models (LLMs), have demonstrated remarkable performance across various domains, including chemistry. [1-4] This study investigates the potential of in-context learning (ICL) in LLMs to predict chemical properties using SMILES-based input data. [5] We designed six chemical property prediction tasks—molecular weight, LogP, sp^3 fraction, topological polar surface area (TPSA), molecular refractivity (MolMR), and graph-based indices (Hall-Kier Alpha, Balaban J, ChIRv)—leveraging the ESOL dataset. [6] Property values were calculated using RDKit, and LLM performance was evaluated under a 50-shot ICL setting, with performance measured via mean absolute error (MAE) and R^2 scores. [7] Our results indicate that LLMs exhibit superior performance compared to traditional machine learning models, particularly in tasks like molecular weight prediction, even without explicit hints. [8] However, performance declines in complex tasks such as Balaban J index prediction, highlighting limitations in capturing intricate structural information. Interestingly, LLMs maintained strong performance regardless of embedding techniques or prompt modifications, suggesting potential retrieval-based reasoning rather than true in-context learning. [9] This study systematically explores the capabilities and boundaries of LLMs in chemical property prediction through ICL. Future research should focus on developing natural language-based molecular representations to overcome SMILES syntax limitations, potentially enhancing prediction accuracy for less well-known properties. Our findings underscore the transformative potential of LLMs in cheminformatics while identifying key areas for further investigation.

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(Poster 20)

Modeling Charge Transfer of Organic Molecules using Multiscale Computational Chemical Methodology

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This study focuses on numerical methods to compute charge carrier mobility solely from molecular structures. While employing the Marcus rate theory in kinetic Monte Carlo (KMC) simulations is suitable for our purposes, it requires precise calculations of the transfer integrals and site energies for specific morphologies. We attempted to extend the current model to a multicharge model, which requires long computation time and faces challenges in calculating site energies. To overcome these limitations, we developed a new lattice mapping method that efficiently obtains transfer integrals and site energies from realistic morphologies, while maintaining a manageable computational cost. Our method was validated by the mobility values computed using the KMC method, which showed strong agreement with the experimental data. Analysis of the charge carrier behavior through residence time calculations provided further insight into the charge transport dynamics. Additionally we demonstrated the applicability of the model to multicharge systems by simulating the exciton formation. In conclusion, our model has the potential to affordably simulate charge carrier trajectories in multicharge, multilayer models with minimal loss of information from the realistic morphology, making it a valuable tool for the design and optimization of organic electronic devices.

(Poster 21)

Investigating Dynamical Phase Transition of Kob-Andersen Model with Trajectory Ensemble Method

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Statistical mechanics of far-from-equilibrium states requires ensemble analysis based on trajectories rather than static configurations. In the trajectory ensemble approach, biasing fields such as the s -field and g -field, which are conjugate to dynamical activity and trajectory energy respectively, serve as essential tools for exploring rare dynamical events and states that are typically inaccessible through conventional methods. We investigate the effect of the g -field on the Kob-Andersen model, a continuous-space binary mixture of Lennard-Jones particles that serves as a representative model for glassy systems. By implementing transition path sampling (TPS) based trajectory sampling through LAMMPS Python API and optimizing the computational framework for sampling efficiency, we successfully constructed two-dimensional phase diagrams in the temperature- g field plane. Our analysis revealed that a well-defined phase transition line terminates at two specific points, indicating the possibility of both upper and lower critical points. This finding provides a novel perspective on the glass transition through the lens of a phase diagram constructed by varying both temperature and the g -field, which are related to trajectory kinetic energy and potential energy respectively, demonstrating that biasing trajectory energy through the g -field provides a unique way to control dynamical activity and potentially bridge thermodynamic and dynamical aspects of glass formation.

(Poster 22)

Elucidating Dynamical Behaviors in Kinetically Constrained Models via Energy-Activity Double-Biased Matrix Product State Analysis

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We investigate dynamical phase transitions in two representative kinetically constrained models: the 1D Fredrickson–Andersen and East Models. A recently developed energy-activity double-bias approach utilizing both s and g fields, conjugated with dynamical activity and trajectory energy, is combined with matrix product state (MPS) methods. It is demonstrated that MPS methods facilitate the numerical approximation of large-deviation statistics of dynamics by determining the eigenvalues of tilted dynamical generators under the influence of double-biasing fields. Specifically, by focusing on the g -field, a nearly “half-filled” state at moderate negative g values is identified, indicating the potential existence of an anomalous phase. Additionally, dynamical quantities under various s , g , and T conditions are obtained via tensor networks, showing good qualitative consistency with mean-field results and our previous extensive numerical simulation results obtained by the path sampling method. Our study introduces novel methodologies for examining decoupled dynamical behaviors that, although energetically active, remain dynamically inactive within the system. This approach offers a fresh perspective on the theoretical framework and computational strategies for studying dynamical phase transitions in kinetically constrained systems. [1]

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(Poster 23)

Ultrastable Glass Sampling via Swap Monte Carlo and Vapor Deposition Monte Carlo

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Ultrastable glass, characterized by its higher density and lower enthalpy compared to conventional glass, exhibits superior mechanical and thermal stability, making it a subject of significant interest. However, its intrinsically slow relaxation presents significant challenges for direct simulation-based studies. In this poster, we explore the efficient generation of ultrastable glass samples using Swap Monte Carlo (SMC) and Vapor Deposition Monte Carlo (VDMC) methods. SMC facilitates deeper supercooled states by reducing structural constraints through particle swaps, thereby accelerating relaxation dynamics. We apply this method to a modified Kob-Andersen, coarse-grained atomistic glass model, by introducing a move set that enables the swapping of two particle positions, enhancing the equilibration process. In contrast, VDMC emulates physical vapor deposition, effectively representing the formation and growth mechanisms of glass. In this poster, multiple molecules are initially deposited as trial configurations, followed by a Monte Carlo selection process based on their energy and Boltzmann distribution, thereby expediting the relaxation dynamics. Furthermore, we implement this approach in a system composed of molecules relevant to amorphous configurations in material research, demonstrating its capability to efficiently identify low-energy molecular arrangements. By comparing and analyzing the thermal and structural properties of the generated samples, we provide deeper insights into the formation pathways and kinetic stability of ultrastable glass. This study establishes a theoretical foundation for optimizing ultrastable glass fabrication under diverse conditions and contributes to further investigations into far-from-equilibrium states, as well as experimental realizations and practical applications.

(Poster 24)

Diffusiophoretic flows in microchannels simulated by a coupled method of Molecular Dynamics and Multiparticle Collision Dynamics

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In experiments one often observes fluid flows in the presence of concentration or temperature gradients on fixed surfaces, for example in glasses or microchannels. These phoretic flows may induce the motions of passive particles and as well play important roles in the dynamics of phoretic particles and thereby their collective behaviors. Here we consider diffusiophoretic flows which arise from the concentration gradients of neutral particles and use a new particle-based simulation method using a coupled method of molecular dynamics and multiparticle collision dynamics to simulate diffusiophoretic flows. Molecular interactions adopted in simulations produce proper no-slip boundary conditions and under an external force Poiseuille flows are created. For a diffusiophoretic flow, the steady state concentration gradients for two chemical species are built along the microchannel. Introducing different interaction potentials between the chemical species and the surfaces, we observed the steady diffusiophoretic fluid flows are indeed created along the channel.

(Poster 25)

Transformer-Based Machine Learning Model for Solvation Free Energy Prediction

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Predicting solvation free energies, especially for non-aqueous solutions, remains a longstanding challenge in physics, chemistry, and biology. Recent studies have proposed leveraging machine learning (ML) strategies such as recurrent neural networks (RNNs) and graph neural networks (GNNs) [1-2]. More recently, the *transformer* architecture, introduced in 2017 [3], has gained significant attention due to its superior performance across various domains, including natural language processing (NLP), computer vision (CV), and cheminformatics. In this study, we explore the application of the transformer architecture to solvation energy prediction. Our findings demonstrate that the transformer architecture can serve as an encoder in ML models for predicting solvation free energies. The results from our transformer-based model show strong agreement with those from previous RNN-based models. Furthermore, we anticipate that optimizing the model structure and fine-tuning its hyperparameters could further improve its predictive accuracy. This approach may also be extended to predict other chemical and physical properties, such as liquid properties, transition state energies, and crystal structures.

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(Poster 26)

Implicit Force Matching: A Unified Approach to Free Energy Surface Estimation from Samples Obtained Across Multiple Ensembles

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Analysis of samples obtained across multiple canonical ensembles to infer free-energy profiles presents a challenge. Maximum likelihood estimation, also known as the Multistate Bennett Acceptance Ratio (MBAR), becomes intractable due to the emergence of multiple normalization constants defined by the free-energy surface model. Thermodynamic integration and its continuous analogs remain tractable; however, they require heuristic approximations, which limit their applicability in general bias potential settings and high-dimensional spaces. Adapting generative models to the joint configuration–control parameter space has emerged as an empirically promising approach, but current approaches lack the use of the bias potential energy information inherent in multi-ensemble data. To fill this gap, we rederive existing free-energy estimators within the framework of joint configuration–control parameter space distribution estimation and the minimum statistical discrepancy principle, providing a unified perspective on generative modeling and free-energy surface estimation, as well as methodological flexibility through the choice of discrepancy. Driven by this perspective, we propose Implicit Force Matching (IFM)—a statistically consistent continuous free-energy estimator. Importantly, inaccurate assumptions in previous thermodynamic integration-based continuous free-energy estimator is eliminated by converting the unknown ensemble average by integration-by-parts, akin to the equipartition theorem and implicit score matching in generative machine learning. We also establish further connections between IFM and bottom-up coarse-graining algorithms by proposing their multi-ensemble generalizations; the asymptotic limit of a generalized relative entropy minimization and a variant of MBAR designed to discriminate between original and infinitesimally translated data. Finally, we analyze asymptotic statistical error and empirically demonstrate this new formalism in estimating the continuous free-energy surface, particularly when using sparse samples.

(Poster 27)

Accelerating Multiscale Simulation of OLED Materials Through Machine Learning

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Organic light-emitting diode (OLED) technology has advanced significantly in recent decades and is now prevalent in devices such as smartphones and TVs, thanks to features such as lower power consumption and high color contrast.^[1] However, the lower efficiency and shorter lifespan of blue OLEDs remain major challenges for researchers.^[2] OLED material research typically employs a screening method that involves synthesizing numerous candidate materials and analyzing them to identify suitable molecules. However, this approach is challenging and time-consuming.^[3] Alternatively, we predict the charge carrier mobility of OLED materials through kinetic Monte Carlo simulation.^[4] The kinetic Monte Carlo method^[5] itself takes little time, but obtaining the parameters, especially transfer integral^[6], needed to calculate the charge transfer rate takes a lot of time. To address this problem, we introduced a machine learning approach to predict transfer integrals without relying on time-intensive DFT calculations.

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(Poster 28)

Multiscale Modeling of OLED Device Operation using Layer-Averaged Space Charge Approach

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Organic light-emitting diodes (OLED) are utilized in the wide range of industry due to its unique advantages. However, designing a new OLED device requires numerous efforts and costs. Multiscale kinetic Monte Carlo (kMC) simulation of devices can be helpful to reduce the cost to develop the new materials and devices, because it provides both microscopic and macroscopic properties of OLED device. Despite the benefits of kMC simulation, it is hard to simulate the whole device operation since it requires high computational cost. In this study, 'extended layer-averaged charge density approach' is proposed, which reduces the cost of inter-charge interaction calculations. By introducing the layer-averaged charge density approach, multiscale kMC simulations of OLED devices are performed on the atomistic morphology and the macroscopic properties such as exciton distribution and voltage-current characteristics are estimated. In conclusion, the model can effectively simulate the OLED device operation. It also has potential to be applied in other organic semiconductor systems like organic photovoltaic solar cells and organic field-effect transistors.

(Poster 29)

Local Excited State Simulation in Periodic System Using MRSF-TDDFT

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In this study, we introduce an advanced methodology for simulating excited states in extended systems by integrating quantum embedding theory with time-dependent density functional theory (TDDFT). To effectively capture electronic momentum in periodic systems, we employ the concept of density matrix embedding theory (DMET) [1-3] to construct an active space within molecular orbitals, encompassing states that are entangled with a specified fragment. We then utilize multi-reference spin-flip TDDFT (MRSF-TDDFT) [4-5] within this active space to achieve high-precision excited state properties. Here, we present example calculation on atomic chain system.

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(Poster 30)

Highly Parallelizable Spatio-Temporal Monte Carlo Sampling Algorithm for Rare Trajectories

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We propose a new Monte Carlo-based method that aims to sample rare or out-of-equilibrium trajectories of the stochastic process. The proposed algorithm is highly parallelizable across both the spatial and temporal dimensions of the given trajectory, which enables far more efficient sampling and provides greater flexibility with respect to various boundary conditions. We also apply the proposed algorithm to the double-biased ensemble of the 1D Ising model. The results demonstrate that the method offers a significantly faster trajectory generation than the traditional shooting/shifting transition path sampling, sufficient to sample the 2D (s , g)-phase diagram of the Ising system. In addition, the proposed algorithm precisely reproduces both the thermodynamic and dynamic behaviors of the system, as predicted by the theoretical approach.

(Poster 31)

Elucidating the Key Factors Governing Reaction Kinetics in Biomolecular Condensates with Emphasis on the Excluded Volume Effect

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Biomolecular condensates are known to enhance reaction kinetics by concentrating reactants; however, factors beyond this mass effect remain largely unexplored. [1-2] In this study, we employed a metal-ion-induced His-tag clustering strategy to trigger protein liquid-liquid phase separation (LLPS) [3] and to investigate the SpyCatcher-SpyTag reaction within these condensates. [4] By utilizing intrinsically disordered protein (IDP) scaffolds (LAF, TAF, and FUS) alongside the folded protein scaffold PRM-SH3 [1, 5], we systematically examined kinetic influences beyond mere reactant recruitment. Our results demonstrate that at high scaffold densities, the excluded volume effect significantly accelerates reaction rates beyond those expected from concentration alone. Notably, diffusivity within the condensates had minimal impact on reaction kinetics; this is attributed to the low reaction rate constant of our SpyCatcher-SpyTag clients, leading to a conformational change-limited reaction rather than a diffusion-limited one. [6] Furthermore, under comparable weight-to-volume density conditions, IDP scaffolds exhibit a more pronounced excluded volume effect than folded proteins, and in densely packed systems, reactants can become isolated, leading to an unreacted fraction. These insights not only deepen our understanding of the multifaceted factors governing reaction kinetics in biomolecular condensates but also highlight the crucial roles of scaffold density and molecular organization, with important implications for the design of synthetic condensate systems and the interpretation of cellular biochemical processes.

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(Poster 32)

(Poster 33)

Metal Substitution in Semi-constrained Systems: DFT Study on a Metalloenzyme

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Metal complexes with constrained or semi-constrained geometry play a crucial role in the coordination chemistry of metalloenzymes by imposing structural limits on the ligands. These constraints result in a pre-distorted coordination geometry, forming an entatic state of the protein. The entatic state of a metalloenzyme directly influences the thermodynamic and kinetic aspects across a broad range of chemical reactions by facilitating faster electron transfer and reaction kinetics. In this work, we selected the catalytic active center of human carbonic anhydrase II (CA II) and its four metal variants containing Co^{2+} , Ni^{2+} , Cu^{2+} , and Zn^{2+} as the model system and conducted a density functional theory (DFT) study on their coordination chemistry. We imposed structural constraints on the active site to mimic the entatic state of the protein and tested various functional and basis set combinations to find the optimal combination for reproducing the experimental structures. We found that the native metal ion in metalloenzymes does not always exhibit the strongest binding, but the trend follows the Irving-Williams series, and that structural constraints make the energy landscape of the metal complexes more rugged. We anticipate that our findings can be utilized to design and tune the entaticity of the active site in artificial metalloenzymes.

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(Poster 34)

Chain Properties of Supercharged Proteins

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Supercharging a protein, by introducing a significant amount of charge, leads to extensive unfolding and stretching of the protein. However, the chain properties of the protein cannot be described by a simple polymer model, mainly due to the conformational constraints in the dihedral space. In this work, we utilized atomistic Monte Carlo simulations to understand the chain properties of supercharged proteins. We focused on proteins with a single intramolecular disulfide bond, which forms a tadpole-like structure after supercharging. We systematically changed the sequence composition and the position of the disulfide bond, spanning various topologies and sequences. By analyzing several measures of the global chain properties, we found that the dihedral angle distribution has no significant effect on determining the chain properties, and that the tail part is more crucial than the ring part for the overall properties. We anticipate that this work will contribute to a deeper understanding of the polymeric features of proteins, and that our findings will be extended to unfolded and intrinsically disordered proteins.

(Poster 35)

Design and Engineering of Phase Separation Driver Proteins

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Liquid-liquid phase separation (LLPS) plays a crucial role in the spatiotemporal compartmentalization of eukaryotic cells, with emerging interest in its underlying mechanisms. A significant subset of LLPS-driving proteins comprises multi-domain proteins characterized by folded domains linked by disordered segments. Based on the established knowledge of LLPS, we designed phase separation drivers by constructing trimers of fluorescent proteins, and investigated their LLPS behaviors. We quantified the phase separation propensity of these trimers through saturation concentration measurements and assessed the material properties of resulting condensates. We compared the LLPS propensity of three fluorescent protein trimers with different binding affinities by measuring their saturation concentration using three distinct methods: turbidity assay, spin-down assay, and imaging assay. Consequently, we observed a correlation between binding affinity and LLPS propensity. We propose that our system can serve as a minimalistic model for investigating the molecular principles of phase separation driver proteins. Our findings contribute to a deeper understanding of LLPS phenomena and may inform the development of strategies for modulating cellular organization and function.

(Poster 36)

Analysis of Intramolecular Network in Protein Structure

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Detailed structural information about a protein is crucial for understanding its function. The structure of a protein is determined by non-covalent interactions between different amino acid residues, and these interactions form an intramolecular network. By analyzing the intramolecular network, the stability and functional characteristics of the protein can be systematically examined. During evolution, protein intramolecular networks adapt in response to physical and biological constraints. Therefore, it is important to understand the general principles governing intramolecular networks of proteins.

In this study, we analyzed the intramolecular networks within protein structures from five phylogenetically distant organisms: a virus, *E. coli*, *Thermoprotei*, *Homo sapiens*, and a mouse. These organisms were chosen due to their distinct features, such as evolutionary rates and widespread use as model organisms in biological research. We examined network topology by dividing the networks into subnetworks and calculating key metrics, such as network size and average degree, which are indicative of the structural complexity and connectivity within the protein. We further explored evolutionary characteristics by calculating sequence space free energy, a measure that reflects the stability and adaptability of protein structures over evolutionary time. Our analysis revealed significant differences in these metrics across the phylogenetically distant organisms, suggesting that the evolution of protein structure is influenced by specific biological and physical constraints unique to each lineage. This study demonstrates the potential of integrating statistical mechanics and network science to deepen our understanding of protein structure evolution.

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Phase Separation of Amino Acid Derivatives and Water: Molecular Dynamics Study

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Biological systems utilize the phase separation of biomolecules in cells. This mechanism plays a crucial role in regulating biological reactions and facilitating the spatiotemporal separation of biomolecules in vivo. Phase separation can induce the local accumulation of particular molecules, hence acting as a catalyst for biological reactions. Thus, it is important to understand the molecular principles of biomolecular phase separation.

To obtain insight into biomolecular phase separation, we employ a simple model system that can undergo phase separation and simulate its phase behavior using molecular dynamics (MD) simulations. The key player in our model system is an amino acid protected by the Fmoc group. The Fmoc-protected amino acid contains both hydrophobic (Fmoc) and hydrophilic (amino acid) groups, and the balance between them can be easily controlled by using different side chains. When mixed with water, the Fmoc-protected amino acid exhibits rich phase behaviors, depending on its side chain.

This study investigates the impact of amino acid polarity on phase separation. By combining molecular dynamics (MD) simulations with the simulated annealing method, we successfully reproduced experimental results and analyzed the phase separation mechanisms driven by polarity differences at the molecular level. Our findings demonstrate that even subtle differences in polarity can significantly influence collective behaviors and phase separation patterns, providing important insights into the principles underlying complex phase separation processes in biological systems. This study highlights how discoveries in simple molecular systems can serve as a foundation for understanding the mechanisms governing biomolecular behavior and offers new directions for research on molecular dynamics.

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Evaluation of Binding Behaviors for Amyloid- β and Tau Inhibitors through Molecular Dynamics Simulations

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The aggregation and accumulation of amyloid- β (A β) and tau are closely associated with the progression of Alzheimer's disease (AD). Inhibiting A β and tau fibrillation and clearing their aggregates have emerged as key therapeutic strategies for AD treatment. Computational methods have become essential tools for drug screening and efficacy prediction. In this study, we employed molecular dynamics (MD) simulations to estimate the efficacy of both experimentally validated A β -inhibitory drugs[1] and non-specific compounds.[2] Docked structures of A β -drug and tau-drug complexes were generated, followed by MD simulations of each system. Interaction analyses were performed using contact probability maps to characterize binding interactions for both A β and tau. Our findings demonstrate the predictive potential of MD simulations in replicating experimental outcomes. This approach underscores the utility of MD-based simulations in accelerating drug discovery efforts targeting A β and tau aggregates.

Reference

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(Poster 39)

Towards Accurate Determination of Binding Free Energy Using Molecular Dynamics Simulations

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The binding free energy between a protein and its ligand partner is crucial for predicting medicinal effects in pharmacology. To computationally obtain binding affinity data, various methods based on molecular dynamics simulations have been developed. Among them, umbrella sampling is a widely used technique for calculating binding free energy by sampling along the association/dissociation process. However, it has been reported that the binding free energy is highly sensitive to the method of sampling; factors such as the initial structure, number of samples, and dissociation path can significantly influence the results. In this work, we performed umbrella sampling with varying sampling time to investigate changes in the potential of mean force (PMF) and its relationship with the number of sampling windows. Our findings indicate that the PMF is influenced by the sampling time. Furthermore, we identified specific window regions that have a pronounced impact on the PMF. Based on these results, we propose a sampling method that enhances the efficiency and reproducibility of PMF calculations. We believe that our method can improve the accuracy of binding free energy estimations, thus contributing to advancements in computational drug design and engineering.

(Poster 40)

One-pot nitridation–exsolution route to high-performance metal nanocluster–metal nitride electrocatalysts

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Exsolution has garnered significant research interest because of its high efficacy in synthesizing metal nanocluster-based composite electrocatalysis.[1] In this study, we report a rationally designed single-step nitridation–exsolution synthetic route to high-performance hydrogen evolution reaction (HER) electrocatalyst.[2] The NH₃ treatment of Ru-substituted oxide nanowires at evaluated temperature induces the exsolution of Ru nanoclusters and also the phase transition to holey metal nitride nanotubes. The obtained Ru exsolved metal nitride nanotube exhibits much higher HER electrocatalytic activity than that of Ru deposited homolog, highlighting the benefit of the nitridation–exsolution approach. The crucial effect of simultaneous nitridation–exsolution process on the HER electrocatalytic activity is attributable to the improved charge transfer kinetics, increased porosity, and the increase of electrocatalytic kinetics. The present study demonstrates that the single-step nitridation–exsolution synthetic strategy can provide an effective means to explore robust composite electrocatalyst materials.

Reference

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(Poster 41)

High-Entropy-Induced Optimization of Electrocatalytic Activity of Inorganic Nanosheets for Hydrogen Production

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High-entropy materials have garnered significant attention because of their versatile functionalities for various renewable energy technologies. Most of high-entropy materials ever-reported could be synthesized by the substitution of diverse metal ions in the solid lattice, which was limited by the accommodability of solid lattice for substituent ions. In this study, an electrostatic force-driven hybridization strategy to explore new concepts of high-entropy materials was developed by employing a set of diverse inorganic nanosheets as hybridization building blocks. The self-assembly of exfoliated MoS₂, WS₂, RuO₂, and reduced graphene oxide (rGO) nanosheets with organic cations enabled to synthesize high-entropy hybrid materials with tailorable crystal structure and electronic configuration. The diversification of nanosheet components was found to be effective in enhancing the electrocatalytic activity of the nanohybrids for hydrogen evolution reaction (HER). In comparison with one-/two-/three-kinds of nanosheet-assembled homologs, the high-entropy nanohybrids with four sets of MoS₂, WS₂, RuO₂, and rGO nanosheets showed much better HER performance with lower overpotential, underscoring the merit of high-entropy host hybridization. The increased electrocatalytic activity of high-entropy self-assembled nanohybrids could be ascribed to the fine-tuning of electronic, morphological, and local structural features of self-assembled nanohybrids. The diversification of host nanosheet layers offered an additional opportunity to further optimize the electrocatalyst performances of high-entropy hybrid materials.