**시스템화학 글로벌 선도연구센터**

**1차년도 동계 학술대회**

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

**장소: 중앙대학교 310 관 B603호 (oral session)**

**중앙대학교 102관 11층 세미나실 (poster session)**

야외, 하늘, 건물, 식물이(가) 표시된 사진

자동 생성된 설명

**주최: 시스템 화학 글로벌 선도연구센터 (GCSC)**

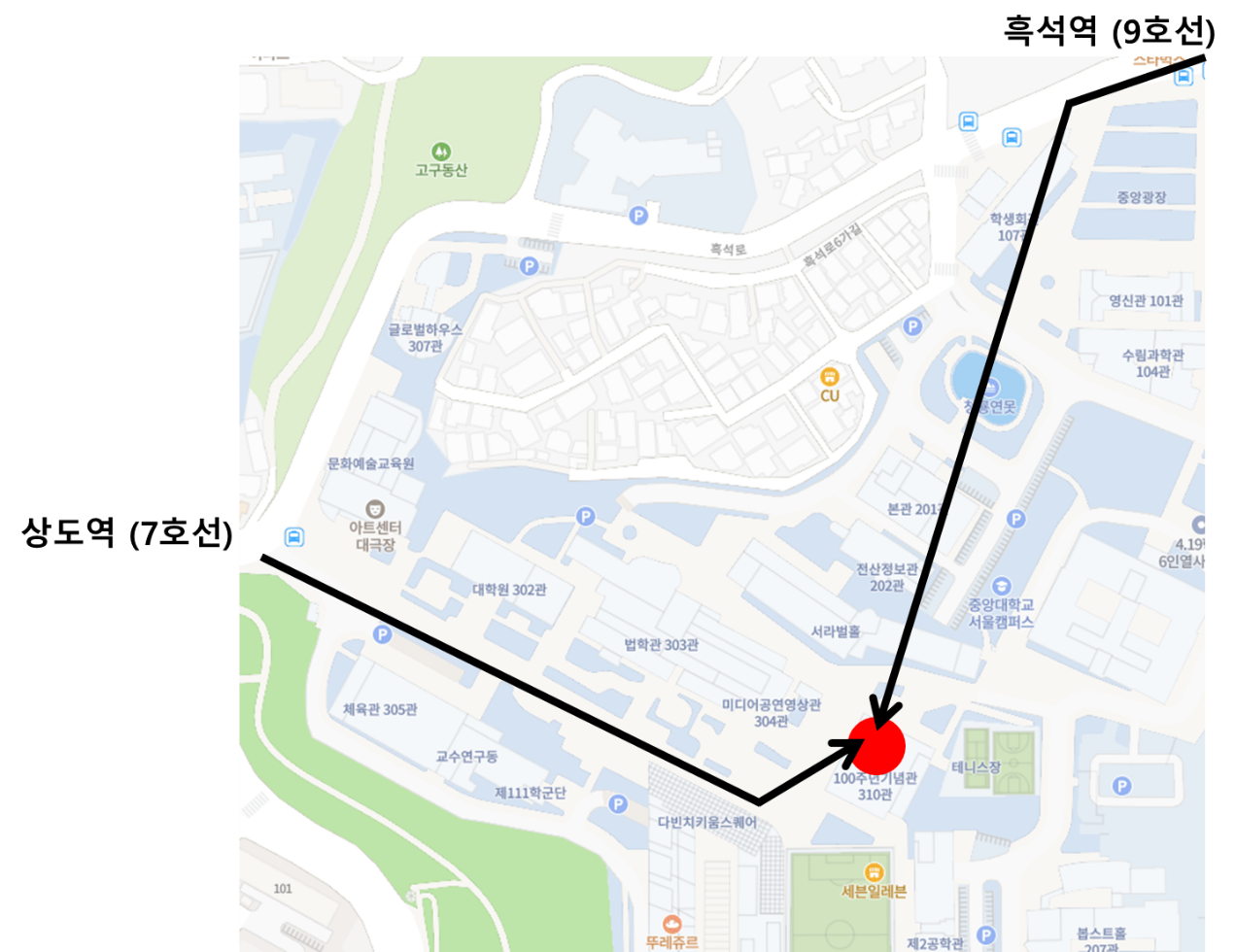
**후원: 중앙대 화학과 BK21 (생물리광화학창의인재양성팀)**

**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**

**2월 25일 (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)** |
| **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)** |
| **10:10~10:20** | **Coffee break** |
| **Session 5 좌장: 고혜란 교수 (중앙대)** | |
| **10:20~10:50** | **이상학 교수 (부산대)** |
| **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**

Name1\*

*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\*

*Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), 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 (Aβ) 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 Aβ plaque and likely contribute to Aβ neurotoxicity and oxidative stress. ROS have been shown to increase the rate of Aβ 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 5-1)**

**Chemical framework for understanding Neurodegenerative Diseases**

Jinmin Lee and Sang Hak Lee1\*

*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**

Name1\*

*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 5)**

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

Sangjin Han1 and Sunmin Ryu1\*

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\*Corresponding e-mail: sunryu@postech.ac.kr

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.

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[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 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\*

*Department of Chemistry, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul,  
 Republic of Korea.*

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 Kim1,2, Seong Jun Park2,3, Ji-Hyun Kim1,2 and Jaeyoung Sung1,2\*

*1Department of Chemistry, Chung-Ang University, Seoul, 06974, Republic of Korea*

*2Creative Research Initiative Center for Chemical Dynamics in Living Cells, 06974 Seoul, Republic of Korea*

*3Department of Physics and Astronomy and Center for Theoretical Physics, Seoul National University, Seoul 08826, Republic of Korea*

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 Kima,b,c, †, Joodeok Kimd,e, †, Byung Hyo Kimd,e,f, †, Sanggeun Songg,h, †, Hoje Chuni, Hyesung Choid,e, Hyungjin Chof, Yongjoon Kimf, Jae Won Jungf, Youngju Sohnd,e, Junhyeok Jeongd,e, Kunwoo Parkd,e, Jinho Rheed,e, Sungho Jeonj, **Jingyu Kang**a,b,c,k, Minho Leea,b,c,k, Byungchan Hani, Won Chul Leej,   
Taeghwan Hyeond,e,\*, Jaeyoung Sunga,b,c,k,\*, Jungwon Parkd,e,l,m,\*

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mAdvanced Institute of Convergence Technology, Seoul National University; Suwon, Gyeonggi 16229, Republic of Korea.* †*These authors contributed equally to this work.  
\*Correspondence regarding experiment should be addressed to jungwonpark@snu.ac.kr (J.P.) and thyeon@snu.ac.kr (T.H.); Correspondence regarding theory should be addressed to jaeyoung@cau.ac.kr (J.S.)*

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 Kang1-3†, Donghee Kim1-3†, Sanggeun Song4,5†, Jonghwa Han1-3, Ji-Hyun Kim1-3\*, and Jaeyoung Sung1-3\*

1 Global Science Research Center for Systems Chemistry, Chung-Ang University, Seoul 06974, Korea.

2 Creative Research Initiative Center for Chemical Dynamics in Living Cells, Chung-Ang University, Seoul 06974, Korea

3 Department of Chemistry, Chung-Ang University, Seoul 06974, Korea.

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5 Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, U.S.A.

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 Lim1,+, **Gyunam Park**1,2,+, Hojin An1,+, Jonghwa Han1,2, Joonhyun Bae3, Ji-Hyun Kim1,2, Yan Lee\* 4, Kyungtae Kang\* 3, Jaeyoung Sung\* 1,2, and Sunbum Kwon\* 1

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2 *Creative Research Initiative Center for Chemical Dynamics in Living Cells, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul 06974, Republic of Korea*

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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.

그림, 일러스트레이션, 만화 영화, 클립아트이(가) 표시된 사진

AI가 생성한 콘텐츠는 부정확할 수 있습니다.

**(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 17)**

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

Janghee Hong1, Rakwoo Chang1\*

*1 Computational Molecular Modeling Laboratory & Department of Applied Chemistry, University of Seoul, Seoul 02504, Korea*

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.

**Reference**

[1] Bryngelson, J. D.; Onuchic, J. N.; Socci, N. D.; Wolynes, P. G. Proteins. 21, 3 (1995).

[2] Day, R.; Daggett, V. Adv. Protein Chem. 66 (2003)

[3] Riniker, S.; Allison, J. R.; van Gunsteren, W. F. Phys. Chem. Chem. Phys. 14, 36 (2012).

**(Poster 19)**

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

Chan Young Joe and Rakwoo Chang\*

*Department of Applied Chemistry, University of Seoul, Seoul 02504, Korea*

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, sp3 fraction, topological polar surface area (TPSA), molecular refractivity (MolMR), and graph-based indices (Hall-Kier Alpha, Balaban J, Chi1v)—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 R2 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.

**Reference**

[1] Vaswani, Shazeer, Parmar, Uszkoreit, Jones, Gomez, Kaiser, and Polosukhin, arXiv (2017).

[2] Jablonka, Schwaller, Ortega-Guerrero, and Smit, Nat. Mach. Intell. **6**, 161 (2024).

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[8] Vacareanu, Negru, Suciu, and Surdeanu, COML (2024).

[9] Nafar, Venable, and Kordjamshidi, arXiv (2024).

**(Poster 33)**

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

Rajeev Kumar, Youngsuk Kim, and Jeong-Mo Choi\*

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*\*Corresponding Author, E-mail:* [*jmchoi@pusan.ac.kr*](mailto:jmchoi@pusan.ac.kr)

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 Co²⁺, Ni²⁺, Cu²⁺, and Zn²⁺ 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.

**References:**

1. Kim *et al.*, Nat. Comm., 11, 4557 (2020).
2. Hoffmann *et al.*, Nat. Che., 10, 355 (2018).
3. Comba *et al.*, Coord. Chem. Rev., 200, 217 (2000).
4. Parr *et al.*, JACS, 121, 1922 (1999).

**(Poster 34)**

**Chain Properties of Supercharged Proteins**

Minseo Kim1, Jongcheol Seo2, and Jeong-Mo Choi1\*

*1Department of Chemistry, Pusan National University, Busan 46241, Korea  
2Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang 37673, Korea*

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.

**(Poster 37)**

**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.

**(Poster 38)**

**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 (Aβ) and tau are closely associated with the progression of Alzheimer’s disease (AD). Inhibiting Aβ 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 Aβ-inhibitory drugs[1] and non-specific compounds.[2] Docked structures of Aβ-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 Aβ 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 Aβ and tau aggregates.

**Reference**

[1] Lee *et al.*, Alz Res Therapy **14**, 177 (2022).

[2] Ruddigkeit *et al.*, J. Chem. Inf. Model. **52**, 2864-2875 (2012)

**(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**

[1] Yun, Jin, and Hwang, Chem. Eng. J. **446**, 136816 (2022).

[2] Yun, Lee, Jin, Soon, and Hwang, Adv. Sci. **11**, 2309819 (2024).

**(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.