

Dynamics and Thermodynamics of Small Biological and Nanomaterial Systems (#PHY006)



**Organizers: Jaeyoung Sung (KCS), Philip Kim (CSC), Seogjoo Jang (ACS),
John Straub (ACS), Peng Chen (ACS)**

Sponsored by: Global SRC for Systems Chemistry

December 16 (Tues)

18:30 ~ 21:00	Reception Rainbow Lanai, Hilton Hawaiian Village
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December 17 (Wed)

Session 1 - Nucleation, Self-Assembly, and Phase Separation	
Chair: Peng Chen	
08:00 ~ 08:25	Hagan Bayley (Univ. of Oxford) Soft functional synthetic tissues and their properties
08:25 ~ 08:50	Joan Shea (UC Santa Barbara) Multiscale simulations of peptide liquid-liquid phase separation
08:50 ~ 09:15	Yongwon Jung (KAIST) Protein Models to Study Dynamics of Biomolecular Liquid-Liquid Phase Separation
09:15 ~ 09:25	Coffee Break
Chair: Joan Shea	
09:25 ~ 09:50	John Straub (Boston Univ.) Exploring the impact of sequence and cellular conditions on amyloid formation and polymorphism
09:50 ~ 10:15	Mi Hee Lim (KAIST) Chemical Strategies to Study Multiple Facets in Alzheimer's Disease
10:15 ~ 10:40	Jaeyoung Sung (Chung-Ang Univ.) Chemical Dynamics, Statistical Thermodynamics, and Transport Theories for Complex Materials and Biological Systems
10:40 ~ 10:50	Coffee Break
Chair: Hagan Bayley	
10:50 ~ 11:15	Joo-Yeon Yoo (POSTECH) Dynamics of Biomolecular Condensates on the ER membrane
11:15 ~ 11:40	Jeong-Mo Choi (Pusan National Univ.) Negative Autoregulation in Biomolecular Condensates

December 17 (Wed)

Session 2 - Dynamics in Living Cells	
Chair: Jaeyoung Sung	
14:00 ~ 14:25	Nam Ki Lee (Seoul National Univ.) Investigation of transcription-translation coupling and quantitative protein-protein interactions in living bacterial cells
14:25 ~ 14:50	Hye Yoon Park (Univ. of Minnesota) Single-molecule imaging of gene expression dynamics in the living brain
14:50 ~ 15:15	Jianshu Cao (MIT) Non-equilibrium Conformational Fluctuations in Driven Chemical Networks
15:15 ~ 15:25	Coffee Break
Chair: Younjoon Jung	
15:25 ~ 15:50	Hongbin Li (U. Brit. Columb) Two-molecule force spectroscopy captures intermolecular misfolding in parallelly organized titin
15:50 ~ 16:15	Ji-Hyun Kim (Chung-Ang Univ.) Age-dependent protein degradation modulates noise of self-regulated gene expression
16:15 ~ 16:40	Tai-Yen Chen (Univ. of Houston) Human transporter de-oligomerization regulates copper uptake into cells
16:40 ~ 16:50	Coffee Break
Chair: Hye Yoon Park	
16:50 ~ 17:15	Guangzhao Mao (Univ. of Edinburgh) Real-time visualization of axonal transport dynamics of protein-gold nanoparticle conjugates in living neurons
17:15 ~ 17:40	I-Ren Lee (National Taiwan Normal Univ.) Slippage Dynamics of Trinucleotide Repeat Hairpins Associated with Neurodegenerative Diseases
17:40 ~ 18:00	Jaroslava Miksovska (Florida International Univ.) Neuronal calcium sensors: target proteins for doxorubicin and paclitaxel and their potential role in neuropathy

December 18 (Thurs)

Session 3 - Materials Science	
Chair: John Straub	
08:00 ~ 08:25	Rigoberto Hernandez (Johns Hopkins Univ.) Dynamical Consistency, Indistinguishability and Data Harvesting in Multi-Scale Material Modeling
08:25 ~ 08:50	Joonkyung Jang (Pusan National Univ.) Molecular Dynamics and Thermodynamics of the Wet Adhesions of Mussel Foot Proteins
08:50 ~ 09:15	Seokmin Shin (Seoul National Univ.) Understanding two faces of self-assembly: amyloid formation & bionanostructure design
09:15 ~ 09:25	Coffee Break
Chair: Rigoberto Hernandez	
09:25 ~ 09:50	Seong-Ju Hwang (Yonsei Univ.) Versatile exsolution routes to energy-functional hybrid materials
09:50 ~ 10:15	Sungho Yoon (Chung-Ang Univ.) Heterogeneous Catalysts Derived from Ru-MACHO Complexes for Highly Efficient CO ₂ Hydrogenation to Formate
10:15 ~ 10:40	YounJoon Jung (Seoul National Univ.) Dynamical Phase Transitions and Charge Transport in Disordered Systems
10:40 ~ 10:50	Coffee Break
Chair: Seong-Ju Hwang	
10:50 ~ 11:15	Cho, Hae Sung (Chung-Ang Univ.) Understanding adsorption of porous crystals
11:15 ~ 11:40	Flanders, Nathan (Univ. of Chicago) Super-Absorption in Silicon Nanocrystals via Ultrafast Anisotropic Disorder

December 18 (Thurs)

Session 4 - Quantum, AI, and Biomolecular Engineering	
Chair: Seogjoo Jang	
13:00 ~ 13:25	Alexandre Tkatchenko (Univ. du Luxembourg) Fluctuating interatomic forces in molecules: Mean decays, but the variance increases with interatomic distance
13:25 ~ 13:50	Seunghoon Lee (Seoul National Univ.) Simulating Photochemical Reactions in Artificial Metalloenzymes
13:50 ~ 14:15	Sunmin Ryu (POSTECH) Molecular Excitons in Two-Dimensional Organic Crystals
14:15 ~ 14:25	Coffee Break
Chair: Ji-Hyun Kim	
14:25 ~ 14:50	Seogjoo Jang (City Univ. of New York - Queens College) Kinetic theory of olfaction and beyond
14:50 ~ 15:15	Philip Kim (Univ. of Toronto) Machine Learning methods for protein and peptide design
15:15 ~ 15:40	Yuqing Qiu (Univ. of Tennessee Knoxville) Thermodynamic Control of Organization and Flow in Cytoskeletal Networks Far Away from Equilibrium: Bridging Simulations and Theory through Machine Learning
15:40 ~ 15:50	Coffee Break
Chair: Philip Kim	
15:50 ~ 16:15	Sang-Hee Shim (Korea Univ.) Independently tunable, resonance stimulated Raman scattering for fluorescence-free single-molecule microscopy
16:15 ~ 16:40	Hye Ran Koh (Chung-Ang Univ.) Single-molecule insights into CRISPR-mediated nucleic acid targeting
16:40 ~ 17:00	Jiayi Huang (Westlake Univ.) Transport Kinetics of Triphenylmethane Dye Molecules at Artificial Liposome Membrane Interfaces by Optical Second Harmonic Generation Scattering

December 18 (Thurs)

Poster session - Exhibit Hall, Hawaii Convention Center	
Board 421	Rakwoo Chang (Univ. of Seoul) Hybrid Resolution Exchange Molecular Dynamics Simulation Methods for Effective Sampling
Board 422	Janghee Hong (Univ. of Seoul) Hybrid Resolution Exchange Molecular Dynamics Simulation Methods for Systems with High Energy Barrier
Board 423	Jiayi huang (Westlake Univ.) Transport Kinetics of Triphenylmethane Dye Molecules at Artificial Liposome Membrane Interfaces by Optical Second Harmonic Generation Scattering
Board 424	In-Chun Jeong (Chung-Ang Univ.) Artificial intelligence-based prediction of septic patient's fate dynamics
Board 425	Sangmin Ji (Chung-Ang Univ.) Visualization of p53 Dynamics in Response to MDM2 Inhibition in Cancer Cells
Board 426	Chan Young Joe (Univ. of Seoul) Evaluating in-context learning in large language models for molecular property regression
Board 427	Jingyu Kang (Chung-Ang Univ.) Multiphasic size-dependent growth dynamics of nanoparticle ensembles
Board 428	Donghee Kim (Chung-Ang Univ.) Supersaturation, Nucleation, and Phase Separation of Mesoscopic Systems
Board 429	Jaeyoung Kim (Pusan National Univ.) Computational Approach to the Identification of Visfatin-Derived Angiogenic Peptides
Board 430	Jinhyung Kim (Chung-Ang Univ.) Quantitative Understanding of Cell Signal Propagation and Adaptative Gene Expression Dynamics: Beyond Classical Systems Biology

Poster session - Exhibit Hall, Hawaii Convention Center	
Board 431	Doo-Hyun Ko (Sungkyunkwan Univ.) Enhancing the Stability and Performance of Organic Bulk-heterojunction Morphology via Multi-Component Blends and Machine Learning Prediction
Board 432	Koichi Kobayashi (Tohoku Univ.) Quantitative analysis of intracellular nucleation of protein crystals
Board 433	Minho Lee (Chung-Ang Univ.) Effects of Divalent Cations on Non-Gaussian Lateral Diffusion of Water Molecules Confined Between Lipid Bilayers
Board 435	Gyunam Park (Chung-Ang Univ.) Counterintuitive Transport and Fusion Dynamics of Synaptic Vesicles in the Presynaptic Terminal of Neurons During Stimulation
Board 436	Jae Hyuk Won (Chung-Ang Univ.) New Chemical Dynamics Framework for Quantifying Bacterial Growth & Persistence
Board 437	Huimo Yang (Chung-Ang Univ.) Chemical fluctuation produced by hierarchical switch: The pivotal role of variability in active state duration