

Frontiers in Computational and Experimental Research on Membranes and Interfaces

A conference celebrating cross-disciplinary research and honoring **Michael Klein** and **Yuen-Ron Shen**

March 19 – 21, 2025

Dr. Poe Lecture Hall, Institute of Atomic and Molecular Sciences, Academia Sinica , Taipei



Program

Time	March 19, 2025 (Wednesday)
8:30-9:00	Registration
9:00-9:15	Opening
Session 1	Chair : Hai-Lung Dai (Temple U)
9:15-9:45	William Jorgensen (Yale U) Evolution of Free-Energy Calculations from Butane to Drug Discovery
9:45-10:15	Vincenzo Carnevale (Temple U) AI Deep Generative Models for Polymer Science
10:15-10:45	David Wu (IoC, AS) Deep Learning Potentials for Modeling Magnesium Oxide Hydration and Structural Transformations
10:45-11:15	Break
Session 2	Chair : Huan-Cheng Chang (IAMS, AS)
11:15-11:45	Hongfei Wang (Westlake U) Pushing the Limit of Sum-Frequency Generation Vibrational Spectroscopy (SFG-VS)
11:45-12:15	Shen Ye (Tohoku U) Experimental Probe on the Interfacial Structures of Functional Materials by SFG Vibrational Spectroscopy
12:15-12:45	Yu-Chieh Wen (IoP, AS) Wavevector-Dependent Nonlinear Optics of Electric Double Layer at Water Interface

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Program

Time	March 20, 2025 (Thursday)
8:30-9:00	Registration
Session 3	Chair : Bruce Yu (IoC, AS)
9:00-9:30	Barry Arkles (Temple U) Ion Flux across Myocardial Cell Membranes as Influenced by Crown and Sialcrown Ethers
9:30-10:00	Yuh-Lin Wang (IAMS, AS) Species Differentiation and Antibiotic Susceptibility Testing of Bacteria Using Surface-Enhanced Raman Spectroscopy
10:00-10:30	Parkson Lee-Gau Chong (Temple U) Biophysical Properties of Archaea Tetraether Lipid Membranes
10:30-11:00	Break
Session 4	Chair : Kuei-Hsien Chen (IAMS, AS)
11:00-11:30	Hrvoje Petek (U Pittsburgh) Nonlinear Spectroscopy with Light and Electrons
11:30-12:00	Ing-Shouh Hwang (IoP, AS) Emerging Picture about Gas Molecules in Water Revealed by Transmission Electron Microscopy
12:00-12:30	Michitoshi Hayashi (CCMS, NTU) First Principle Simulation Study of Vibrational Spectra of Materials
12:30-14:00	Lunch
Session 5	Chair : Pei-Kuen Wei (RCAS, AS)
14:00-14:30	Balasubramanian Sundaram (JNCASR) Modeling Chiral Induction from Chiral Surfaces to Achiral Dyes
14:30-15:00	Wataru Shinoda (Okayama U) Heterogeneity of Multicomponent Lipid Membranes
15:00-15:30	Chun-Wei Pao (RCAS, AS) Extensive Microstructure Sampling of Perovskite Films from Machine Learned Energy Models
15:30-16:00	Break
Session 6	Chair : Heng-Liang Wu (CCMS, NTU)
16:00-16:30	Yi Rao (Utah State U) Development of Interface-Specific Two-Dimensional Vibration-Electronic Spectroscopy for Vibrational Couplings at Surfaces and Interfaces
16:30-17:00	Akihiro Morita (Tohoku U) Microscopic Pictures of Ion Transport through Liquid-Liquid Interfaces
17:00-17:30	Eric Borguet (Temple U) The Interfacial Dielectric Constant
18:30	Banquet (by invitation)

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Program

Time	March 21, 2025 (Friday)
8:30-9:00	Registration
Session 7	Chair : Ching Cheng (NCKU)
9:00-9:30	Chao-Ping Hsu (IoC, AS) Excited-State Charge Transfer Coupling from Quasiparticle Energy DFT
9:30-10:00	Chia-Lung Hsieh (IAMS, AS) Single-Molecule Membrane Dynamics at the Nanoscale
10:00-10:30	Michael Klein (Temple U) Water Water Everywhere
10:30-11:00	Break
Session 8	Chair : Ru-Pin Pan (NYCU)
11:00-11:30	Juen-Kai Wang (CCMS, NTU) Enhancement Factor and Continuum Background of Surface-Enhanced Raman Scattering
11:30-12:00	Chi Chen (RCAS, AS) Imaging and Manipulation of Phase-Separated Lipid Bilayers by Scanning Near-Field Optical Microscopy
12:00-12:30	Yuen-Ron Shen (UC Berkeley) Surface Nonlinear Optical Spectroscopy for Membranes
12:30-12:45	Closing