[TS13F6]

AI and Computational Science Based Smart Nanomaterials 6

Date & Time	July 10(Fri.), 2026 / 09:30-11:00
Place	Room 213
Session Chair(s)	Prof. Joonhee Kang (Pusan National University)

TS13F6_O_1 09:30-09:45

Flexible Hofmann-Type Metal-Organic Frameworks for Xe Storage: Machine Learning Potential-Based Molecular Dynamics Approach

Dong Yun Shin[1], Hyojin Kim[2], Chang Seop Hong[3], and Jung-Hoon Lee[1,4]
([1]Korea Institute of Science and Technology, [2]Sookmyung Women's University, [3]Korea University, [4]KU-KIST)

TS13F6_O_2 ***YSA Applied** 09:45-10:00

Electric Double Layer Structure in Concentrated Aqueous Solution

Minho M. Kim and Hyungjun Kim
(Korea Advanced Institute of Science and Technology)

TS13F6_O_3 ***YSA Applied** 10:00-10:15

Water-Mediated Stabilization of Oxyl Radicals as Driving Force for the Oxygen Evolution Reaction

Jaewoo Jeong[1], Hyungjun Kim[1], and Hyeyoung Shin[2]
([1]Korea Advanced Institute of Science and Technology, [2]Kyung Hee University)

TS13F6_O_4 10:15-10:30

Data-Driven Rational Design of Electrolyte Additives via a Dual-Loop Active Learning Framework

Ho Yeon Jang[1] and Seoin Back[2,3,4]
([1]Sogang University, [2]KU-KIST, [3]Korea University, [4]Ewha Womans University)

TS13F6_O_5 ***YSA Applied** 10:30-10:45

Unlocking the $Li_7M_3X_2O_{12}$ Garnet Electrolyte Landscape with Universal Machine Learning Interatomic Potentials

Mingyu Jeon[1], Donghun Kim[2], and Jung-Hoon Lee[1,3]
([1]Korea Institute of Science and Technology, [2]Korea Advanced Institute of Science and Technology, [3]KU-KIST)

TS13F6_O_6 ***YSA Applied** 10:45-11:00

Predicting Plateau Slope in Metal Hydrides from First-Principles: Hydrogen Energy and Charge Distributions in $TiMn_2$-Based Alloys

Jae Hur[1], Ryun-Ho Kwak[2], Seo-Hui Park[1], Tae-Wook Na[2], Hyung-Ki Park[2], and Won-Seok Ko[1]
([1]Korea University, [2]Korea Institute of Industrial Technology)