[TS13F7]

AI and Computational Science Based Smart Nanomaterials 7

Date & Time	July 10(Fri.), 2026 / 14:00-16:30
Place	Room 213
Session Chair(s)	Dr. Jung-Hoon Lee (KIST)

TS13F7_O_1 ***YSA Applied** 14:00-14:15

Molecular Dynamics Study of Tramp Element Effects on Liquid Metal Penetration in Fe-Cu-X Ternary Systems

Jong-Hoon Park[1], Hye-Ji Jo[1], Hye-Hyun Ahn[1], Dong-Hwi Kim[2], Min-Woo Kang[2], Youngjae Kim[2,3], and Won-Seok Ko[1]
([1]Korea University, [2]Hyundai Motor Company, [3]Seoul National University)

TS13F7_O_2 ***YSA Applied** 14:15-14:30

Solomon: Toward an AI Co-Scientist for Battery Materials

Jisu Kim[1], Hyunsung Cho[1], Haekwan Jeon[1], Euitae Lee[1], Seyong Im[1], and Seungwu Han[1,2]
([1]Seoul National University, [2]Korea Institute for Advanced Study)

TS13F7_O_3 14:30-14:45

Predicting CO_2 Reduction Selectivity on Large-Scale Cu-Pd Nanoparticles via a Multi-Scale Machine Learning Framework

Wooseok Lee[1] and Seoin Back[2,3]
([1]Sogang University, [2]KU-KIST, [3]Korea University)

TS13F7_O_4 ***YSA Applied** 14:45-15:00

Multi-Objective Discovery of Cost-Effective and Durable OER Catalysts for PEM Water Electrolysis via Self-Driving Lab

Daeho Kim[1,2], Hyobin Nam[3], Sae Yane Paek[1], Nayeon Kim[1,2], Heeseung Lee[1,2], Hyuk Jun Yoo[1], Sang Kyu Kwak[2], Jong Min Kim[1,3], Seung Yong Lee[1], and Sang Soo Han[1]
([1]Korea Institute of Science and Technology, [2]Korea University, [3]Kyung Hee University)

TS13F7_O_5 ***YSA Applied** 15:00-15:15

Vacancy-Induced Dynamic Evolution of Cu Dual-Atom Sites Enables C-C Coupling for Electrochemical CO_2/CO Reduction

Hyun Dong Jung[1] and Seoin Back[2]
([1]Sogang University, [2]Korea University)

TS13F7_O_6 15:15-15:30

Active Learning of Synthetically Constrained High-Entropy Oxide

Min Young Ha
(Kyung Hee University)

TS13F7_O_7 ***YSA Applied** 15:30-15:45

Efficient Design of Multi-Objective Seawater Electrolysis Catalysts Using an Active Learning Framework for High-Entropy Alloys

Kwangsoo Kim[1], Byung-Hyun Kim[2], and YongJoo Kim[1]
([1]Korea University, [2]Hanyang University ERICA)

TS13F7_O_8 ***YSA Applied** 15:45-16:00

Solvation Structure Modulation in Aqueous Electrolytes: Stabilizing Pyrazine Radicals and Facilitating Electrochemical Nitrate Reduction

Min Young Seo[1], Seeun Hong[2], Cheolmin Park[2], Jinho Chang[2], and YongJoo Kim[1]
([1]Korea University, [2]Hanyang University)

TS13F7_O_9 ***YSA Applied** 16:00-16:15

Data-Driven Discovery of Oxide Electrolytes for Na-Ion All Solid-State Batteries

Atefeh Yadegarifard[1,2] and Byungju Lee[1,2]
([1]Korea Institute of Science and Technology, [2]University of Science and Technology)

TS13F7_O_10 16:15-16:30

Fine-Tuned Large Language Models for MOF Diagnosis and Recovery

Xiao-Yan Li
(National University of Singapore)