[TS13T3]

AI and Computational Science Based Smart Nanomaterials 3

Date & Time	July 9(Thu.), 2026 / 09:30-11:00
Place	Room 213
Session Chair(s)	Prof. Donghun Kim (KAIST)

TS13T3_O_1 ***YSA Applied** 09:30-09:45

LLM-Driven Synthesis Planning for Inorganic Materials Discovery

Dong Won Jeon and Sung Beom Cho
(Ajou University)

TS13T3_O_2 ***YSA Applied** 09:45-10:00

Machine Learning Interatomic Potential-Driven Multiscale Modeling of Interfacial Water Dynamics on Electrocatalytic Surfaces

Miyeon Kim and Jeong Woo Han
(Seoul National University)

TS13T3_O_3 10:00-10:15

Benchmarking a Pretrained Universal MLIP on Energy Materials: Realistic Modelng and Potential-Aware Simulations

Jinwoong Chae[1], Hyeseung Kim[1], Hyun-Jae Lee[1], Sojeong Yang[1], Kiseop Im[1], Yang-Jun Lee[2], Jungwoo Choi[1], Byung Chul Yeo[3], Donghun Kim[4], Sang Soo Han[1], Byungju Lee[1,5], Stefan Ringe[6], and Sungwoo Kang[1,5]
([1]Korea Institute of Science and Technology, [2]Seoul National University, [3]Pukyong National University, [4]Korea Advanced Institute of Science and Technology, [5]University of Science and Technology, [6]Korea University)

TS13T3_O_4 ***YSA Applied** 10:15-10:30

Understanding Precipitation Behavior in Cu-Ni-Si-Mn Alloys Using Machine-Learning Interatomic Potential Calculations

Aadil Fayaz Wani[1], Il-Seok Jeong[2], SuDong Park[1], Eun-Ae Choi[2,3], Sueng Zeon Han[2,3], and Byungki Ryu[1,3]
([1]Korea Electrotechnology Research Institute, [2]Korea Institute of Materials Science, [3]University of Science and Technology)

TS13T3_I_5 ***Invited** 10:30-11:00

Leveraging Generative AI and Agents for Catalyst Discovery

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(Korea University)