[TS13W1]

AI and Computational Science Based Smart Nanomaterials 1

Date & Time	July 8(Wed.), 2026 / 09:30-11:00
Place	Room 213
Session Chair(s)	Prof. Min Young Ha (Kyung Hee University)

TS13W1_O_1 ***YSA Applied** 09:30-09:45

Data-Driven Prediction and Interpretation of Photocatalytic Dye Degradation by Anatase TiO_2 Nanorods under Natural Sunlight: Capturing Diurnal Variability Using Machine Learning

Pravenraam Shankar, Sanjhana Anandan, Vairamuthu Subbiah, and Selva Rani Balasubramaniam
(Vellore Institute of Technology)

TS13W1_O_2 ***YSA Applied** 09:45-10:00

Data-Efficient Active Learning for Accelerated Discovery of Water Electrolysis Catalysts

Junseok Moon[1,2] and Taeghwan Hyeon[1,2]
([1]Seoul National University, [2]Institute for Basic Science)

TS13W1_O_3 10:00-10:15

Understanding Oxygen Ion Transport Mechanisms in Next-Generation Solid Oxide Electrolytes via Machine Learning Potentials

Jisoo Nam and Byungju Lee
(Korea Institute of Science and Technology)

TS13W1_O_4 ***YSA Applied** 10:15-10:30

SevenNet-Omni: A Universal Machine Learning Interatomic Potential for Unified Molecular and Materials Simulations

Jinmu You[1], Jaesun Kim[1], Yutack Park[1], Yunsung Lim[1], Haekwan Jeon[1], Suyeon Ju[1], and Seungwu Han[1,2]
([1]Seoul National University, [2]Korea Institute for Advanced Study)

TS13W1_O_5 ***YSA Applied** 10:30-10:45

Multiscale Simulation of Dynamic Pt Nanoparticle Reconstruction on Facet-Engineered TiO_2 Using Neural Network Potentials

Yunkyung Kim and Jeong Woo Han
(Seoul National University)

TS13W1_O_6 10:45-11:00

Structural Necessity of Monoclinic $P2_1/c$ Phase via Phonon-Mode Coupling at Ferroelectric Domain Boundaries in HfO_2

Hyun-Jae Lee
(Korea Institute of Science and Technology)