[TS13T5]

AI and Computational Science Based Smart Nanomaterials 5

Date & Time	July 9(Thu.), 2026 / 15:50-17:50
Place	Room 213
Session Chair(s)	Prof. YongJoo Kim (Korea University)

TS13T5_O_1 ***YSA Applied** 15:50-16:05

Physics-Informed Graph Neural Network for CO_2 Reduction Electrocatalyst Discovery

Jihoon Kim and Yun Jeong Hwang
(Seoul National University)

TS13T5_O_2 16:05-16:20

Design of Sc-Alloyed RuO_2 Nanomaterials for High-Performance and Durable Acidic Water Electrolysis

Soonsung So and Sang Soo Han
(Korea Institute of Science and Technology)

TS13T5_O_3 ***YSA Applied** 16:20-16:35

Interfacial Cooperation-Driven Volcano Shifts in Ammonia Decomposition Revealed by Reaction-Aware Machine Learning Simulations

Jungwoo Choi[1], Sungwoo Kang[1,2], Byung Chul Yeo[3], and Donghun Kim[4]
([1]Korea Institute of Science and Technology, [2]University of Science and Technology, [3]Pukyong National University, [4]Korea Advanced Institute of Science and Technology)

TS13T5_I_4 ***Invited** 16:35-17:05

Towards Realistic Simulations of Electrocatalytic Interfaces Using Neural Network Models

Nitish Govindarajan
(Nanyang Technological University)

TS13T5_I_5 ***Invited** 17:05-17:35

Ru Oxidation State Governs Competing Oxygen Evolution and Dissolution Pathways on RuO_2 in Water

Chao Yang and Pengfei Ou
(National University of Singapore)

TS13T5_O_6 17:35-17:50

Decoding Ensemble Effects of Multimetallic Active Sites via Surrogate Models and Active Learning

Hoje Chun
(Kookmin University)