# [TS13T4]

## AI and Computational Science Based Smart Nanomaterials 4

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| Date & Time | July 9(Thu.), 2026 / 14:00–15:30 |
| Place | Room 213 |
| Session Chair(s) | Prof. Sung Beom Cho (Ajou University) |

TS13T4_O_1 ***YSA Applied** 14:00–14:15

**The Effect of B-Site Element on Proton Conductivity in $ABO_{2.5}$ Brownmillerite Structures: A First-Principles Study**

Suyun Chae, Eunji Ahn, Yonghun Shin, June Ho Lee, Hyomin Hong, and Donghwa Lee
(Pohang University of Science and Technology)

TS13T4_O_2 ***YSA Applied** 14:15–14:30

**A Robust Agentic Framework for Expert-Level Automation of Atomistic Simulations**

Yutack Park[1], Yeonwoo Chung[1], Jinmu You[1], and Seungwu Han[1,2]
([1]Seoul National University, [2]Korea Institute of Advanced Study)

TS13T4_I_3 ***Invited** 14:30–15:00

**Statistical Mechanics Based Catalyst Designs: Computations and Experiments**

Heechae Choi
(Xi'an Jiaotong-Liverpool University)

TS13T4_I_4 ***Invited** 15:00–15:30

**Stabilizing Metastable Defects in Wide-Band-Gap Semiconductors**

Kai Liu, Chenxi Nie, Wentao Ou, and Guangfu Luo
(Southern University of Science and Technology)