# [TS13W2]

## AI and Computational Science Based Smart Nanomaterials 2

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| Date & Time | July 8(Wed.), 2026 / 15:50-17:35 |
| Place | Room 213 |
| Session Chair(s) | Prof. Doosun Hong (University of Seoul) |

TS13W2_O_1 ***YSA Applied** 15:50-16:05

**Effective Carbide Interface Engineering to Mitigate Hydrogen Embrittlement: A First-Principles Study**

Changhun Kim, Seon-Gyu Kim, Shinhyun Kim, Seungyoun Jo, and Donghwa Lee
(Pohang University of Science and Technology)

TS13W2_O_2 ***YSA Applied** 16:05-16:20

**Beyond Classical Nucleation: A Coupled-Flux Framework for Predictive Polymorph Selection, Demonstrated in $TiO_{2-x}$**

Han Uk Lee and Sung Beom Cho
(Ajou University)

TS13W2_O_3 ***YSA Applied** 16:20-16:35

**Exploring the Impact of Amorphous Conditions on Phase Stability in Atomic Layer Deposition Process**

Min Sung Kang and Sung Beom Cho
(Ajou University)

TS13W2_I_4 ***Invited** 16:35-17:05

**Facet-Dependent Catalytic Activity of Rutile $IrO_2$ for the Oxygen Evolution Reaction**

Soonho Kwon
(Pohang University of Science and Technology)

TS13W2_O_5 ***YSA Applied** 17:05-17:20

**First-Principles Investigation of Point Defects and Doping in $Si_2Te_3$ for Electronic Applications**

Youngjun Park, Jaeseon Kim, June Ho Lee, and Donghwa Lee
(Pohang University of Science and Technology)

TS13W2_O_6 ***YSA Applied** 17:20-17:35

**Chemically Intuitive Equivariant Graph Neural Networks for Directional Property Learning**

Jihoo Kim and Hyungjun Kim
(Korea Advanced Institute of Science and Technology)