

[TS16F7]

Computational Materials and Data Science for Nanotechnology 7

Date & Time	July 5(Fri.), 2024 / 14:00–15:40
Place	Room 213
Session Chair(s)	Minkyu Park (Virtual Lab Inc.)

TS16F7_O_1 14:00–14:20

Data/AI-Enabled Acceleration of Catalyst Development

Donghun Kim
(KIST)

TS16F7_O_2 14:20–14:40

Data-Driven Anomaly Classification of Molecule-Adsorbed Catalyst Surfaces

Juhwan Noh and Hyunju Chang
(KRICT)

TS16F7_O_3 14:40–14:55

Introduction to SevenNet

Seungwoo Hwang, Yutack Park, Jaesun Kim, and Seungwu Han
(Seoul National University)

TS16F7_O_4 14:55–15:10

Inverse Design for Materials Discovery from the Multidimensional Electronic Density of States

Doosun Hong¹, Kihoon Bang¹, Jeongrae Kim^{1,2}, Donghun Kim¹, and Sang Soo Han¹
(¹KIST, ²Korea Polytechnics)

TS16F7_O_5 15:10–15:25

A Combined First-Principles and Machine Learning Exploration of Alloying the Lithium Metal Anode for Enhanced Li-S Battery Performance

Il Seok Jeong, Seung Zeon Han, and Eun Ae Choi
(KIMS)

TS16F7_O_6 15:25–15:40

Unveiling 3D Structural Information via Deep Learning of 4D-STEM

Jinho Byun¹, Keeyong Lee¹, Daesung Park², Hyobin Yoo², Geun Ho Gu¹, and Sang Ho Oh¹
(¹KENTECH, ²Sogang University)