

[TS16T5]**Computational Materials and Data Science for Nanotechnology 5**

Date & Time	July 4(Thu.), 2024 / 15:40–18:05
Place	Room 213
Session Chair(s)	Hyun You Kim (Chungnam Nat'l Univ.)

TS16T5_I_1 *Invited 15:40–16:10**Computational Catalysts Design for the Sustainable Hydrogen Future**Xiangfu Niu¹, Shuwei Li¹, and Liang Zhang^{1,2}*(¹Tsinghua University, ²Beijing Huairou Laboratory)***TS16T5_O_2 16:10–16:30****Simulation of Catalyst Degradation using Machine-Learned Potentials**Sungwoo Kang¹, Jisu Jung², Suyeon Ju², Purun-hanul Kim², Deokgi Hong², Wonseok Jeong³, and Seungwu Han²*(¹KIST, ²Seoul National University, ³Lawrence Livermore National Laboratory)***TS16T5_O_3 16:30–16:50****Constructing a Knowledge-Centric Vector Database for Materials Science: Bridging Data, Information, and Insights**

Jungho Shin

*(KRICT)***TS16T5_O_4 16:50–17:05****Unlocking Design Strategies for Oxygen Evolution Reaction Catalysts: Insights from Kinetic Perspective via Constrained Ab Initio Molecular Dynamics Simulations**

Dongyup Shin and Sang Soo Han

*(KIST)***TS16T5_O_5 17:05–17:20****Design Strategies of Bimetallic Catalysts for Electroreduction of Toluene into Methylcyclohexane**

Chen-Hui Chan and Sang Soo Han

*(KIST)***TS16T5_O_6 17:20–17:35****Studying Facet-Selective Adsorption of CO on Cu using the Random Phase Approximation**

Seungchang Han and Stefan Ringe

(Korea University)

TS16T5_O_7

17:35–17:50

Rational Design of Graphene-Supported Single-Atom Catalysts via Formulating Electronic Descriptors for Oxygen Electrocatalysis

Jungwoo Choi^{1,2}, Doosun Hong², and Hyuck Mo Lee¹

(¹KAIST, ²KIST)

TS16T5_O_8

17:50–18:05

DFT Investigation of CO₂ Hydrogenation on Pd-Based Catalysts: Exploring the Impact of C–O Bond Activation

Yejung Choi, Hyuk Choi, Ju Hyeok Lee, Jongseok Kim, and Hyun You Kim

(*Chungnam National University*)

NANO
KOREA
2024
Symposium