

Session Code	[07] ThD1
Session Title	AI-Assisted Design of Functional Materials
Date and Time	Thursday, October 7, 2021 / 10:40-11:45
Session Room	Room D (302)
Session Chair(s)	Jeongwoo Han (POSTECH, Korea) Ki-Ha Hong (Hanbat Nat'l Univ., Korea)

[[07] ThD1-1] Invited Talk **10:40-11:05**
Catalyst Design for Nitrogen and Oxygen Reduction Reactions by Deep Learning

Sang Soo Han, Donghun Kim (*KIST, Korea*), Youngtae Park, and Hyuck Mo Lee (*KAIST, Korea*)

[[07] ThD1-2] Invited Talk **11:05-11:30**
AI-Driven Materials Design

Kyung-Yeon Doh, Seongyu Kim, Shin Hyun Kim, Eunji Ahn, and Donghwa Lee (*POSTECH, Korea*)

[[07] ThD1-3] **11:30-11:45**
Adsorption Energy and Surface Pourbaix Diagram of Metal Nanoparticles: Prediction by Crystal Graph Convolutional Neural Network

Kihoon Bang (*KIST, Korea*), Youngtae Park (*KAIST, Korea*), Donghun Kim (*KIST, Korea*), Hyuck Mo Lee (*KAIST, Korea*), and Sang Soo Han (*KIST, Korea*)