Oct. 6, 2021 (Wednesday)

Session Code	[07] WeD1
Session Title	Computational Catalyst Design 1
Date and Time	Wednesday, October 6, 2021 / 10:00-11:20
Session Room	Room D (302)
Session Chair(s)	Hyun You Kim (Chungnam Nat'l Univ., Korea)
	Jeongwoo Han (POSTECH, Korea)

[[07] WeD1-1] Invited Talk   [Online] 10:00-10:25

Machine Learning Simulation using LASP: Current Status, New Development and Connection with Catalysis Experiment

Zhipan Liu *(Fudan Univ., China)*

[[07] WeD1-2] Invited Talk   [Online] 10:25-10:50

Towards the Computational Design of Core-Shell Nanoparticle Catalysts

Liang Zhang *(Tsinghua Univ., China)*

[[07] WeD1-3]   10:50-11:05

Atomic Precision Design of Highly-Reactive Single-Atom Catalysts through Interface Engineering

Hyuk Choi, Ju Hyeok Lee, and Hyun You Kim *(Chungnam Nat'l Univ., Korea)*

[[07] WeD1-4]   11:05-11:20

Density Functional Theory Study of the Pronounced Effect of Sn on RhSn Catalysts for Propane Dehydrogenation

Seokhyun Choung and Jeong Woo Han *(POSTECH, Korea)*