

[TS16T3]**Computational Materials and Data Science for Nanotechnology 3**

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| Date & Time | July 4(Thu.), 2024 / 09:00–10:35 |
| Place | Room 213 |
| Session Chair(s) | Dong-Hwa Seo (KAIST) |

TS16T3_I_1 *Invited 09:00–09:30**Predicting Polaron Stabilities and Barriers in Battery Materials**

Harald Oberhofer

*(University of Bayreuth)***TS16T3_O_2 09:30–09:50****Highly Reliable and Large-Scale Simulations of Argyrodite Solid-State Electrolytes using a Machine-Learned Moment Tensor Potential**

Ji Hoon Kim, Ji Seon Kim, and Sang Uck Lee

*(Sungkyunkwan University)***TS16T3_O_3 09:50–10:05****Revealing Interfacial Superionic Conduction Mechanisms of New Halide Nanocomposite Solid Electrolytes for All-Solid-State Batteries**Jae-Seung Kim¹, Hiram Kwak², Daseul Han³, Kyung-Wan Nam³, Yoon Seok Jung², and Dong-Hwa Seo¹*(¹KAIST, ²Yonsei University, ³Dongguk University)***TS16T3_O_4 10:05–10:20****Phase-Field Modelling of Electrodeposition in Aqueous Zn Ion Batteries**

Mohan Dasari, Arijit Roy, John Hong, and Pil-Ryung Cha

*(Kookmin University)***TS16T3_O_5 10:20–10:35****Prediction of Degradation in Li-Metal Anodes over Charging/Discharging Cycles**

Hyunjoo Lee and Dongchoul Kim

(Sogang University)