

[TS16W2]**Computational Materials and Data Science for Nanotechnology 2**

Date & Time	July 3(Wed.), 2024 / 15:40–18:00
Place	Room 213
Session Chair(s)	Ji Woong Yu (KIAS)

TS16W2_I_1 *Invited 15:40–16:10**Molecular Dynamics Study on (Poly)electrolytes**

Chanui Park, Seulwoo Kim, Junbeom Cho, Minhwan Lee, Sebin Kim, Sang Deok Kim, and Won Bo Lee
(*Seoul National University*)

TS16W2_O_2 16:10–16:30**Understanding Novel Nano Structures and Anomalous Dynamics Induced by Strong Confinement and Surface Polarization with Molecular Simulations**

Chang Yun Son
(*POSTECH*)

TS16W2_O_3 16:30–16:45**Designing Fluorinated Polymers with High Glass Transition Temperature using Machine Learning Models**

Jin-Hoon Yang, Jiyoung Lee, Hajin Kwon, Eun-Ho Sohn, Hyunju Chang, and Seunghun Jang
(*KRICT*)

TS16W2_O_4 16:45–17:00**Efficient and Transferable Many-Body Noncovalent Interaction Model for Water: The SAPT-MLW**

Kyeong-Jun Jeong and Chang Yun Son
(*POSTECH*)

TS16W2_O_5 17:00–17:15**Understanding Lower Dielectric Constant and Anomalous Dynamics in Nanoconfined Water**

Chaemin Jeong and Chang Yun Son
(*POSTECH*)

TS16W2_O_6 17:15–17:30**Computational Study of Lithium Ion-Transport in Covalent Organic Frameworks**

Akshay Gurumoorthi and Chang Yun Son
(*POSTECH*)

TS16W2_O_7

17:30-17:45

Two Fates of Peptide Isomerization Kinetics Near Aqueous Interfaces

Sangmin Lee and Chang Yun Son

(POSTECH)

TS16W2_O_8

17:45-18:00

First Principle Force Field for the Lithium Ion Battery Electrolytes

Seungwon Jeong and Chang Yun Son

(POSTECH)

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