International Workshop on Advanced Methods for Nano Materials Design

Satellite Session of Nano Korea 2017 Symposium

July 14, 2017, KINTEX, Gyeonggi-do, Korea

This one day workshop is organized by the joint project team to develop the platforms for functional nano particles and the core/advanced technology for computational nanoscience platforms. The workshop will focus on the advanced materials design tools that can strengthen the capability of the nanomaterials design platform.

Following topics will be extensively discussed in this invited-only workshop.

- Global Scale Database of Computational Materials Properties
- Present Status of Materials Big Data and Materials Informatics
- Computational Nanoscience Platform
- Automated Force Field Development
- Accelerated Molecular Dynamics Simulation and its Applications
- Efficient Methods for Electronic Structure Calculation
- QM/MM hybrid method for Electro-chemical Reaction Simulation
- Simulations in Extreme Scale

8:00 Registration

9:00-9:30 (Opening and Introduction) “Development of Thematic Materials Design Platforms”

Kwang-Ryeol Lee and Seungchul Kim

Korea Institute of Science and Technology, Korea

9:30-10:00 (Invited-1) “Accelerating Materials Discovery with Data-driven Atomistic Computation Tools”

Chris Wolverton

Northwestern University, USA

10:00-10:30 (Invited-2) “A New Molecular Design Based on Bayesian Inference and First-Principles Simulations”

Kenta Hongo

Japan Advanced Institute of Science and Technology, Japan

10:30-11:00 Break

11:00-11:30 (Invited-3) “Recent Advances in Non-adiabatic Molecular Dynamics Simulations of Nanoscale Materials”
Oleg Prezhdo
University of Southern California, USA

11:30-12:00 (Invited-4) “Recent Development in Accelerated Molecular Dynamics Methods”
Art Voter
Los Alamos National Lab., USA

12:00-12:30 (Poster Presentation) 3 min for each poster
Poster-1 : “Concept of Thematic Platform for Electrochemistry” (Seungchul Kim, KIST)
Poster-2 : “Prediction of Shape, Atomic Distribution and Structural Stability of Nano Particle Catalyst” (Byeong-Joo Lee, POSTECH)
Poster-3 : “OORI-QNANO: An Effective Mass Approach Code for the Design of Semiconductor Nanostructures for Optoelectronic Applications” (Yonghoon Kim, KAIST)
Poster-4 : “Automation of DFT Calculations of Molecular Surface Reaction on Metal Alloys” (Chanwoo Lee, KIER)
Poster-5 : “Contents Management System for Nano Materials Design Platform” (Minho Lee, Virtual Lab Co., Ltd, and Kwang-Ryeol Lee, KIST)
Poster-6 : “Theoretical Core-level Spectroscopy of Metals and Their Oxide Surfaces” (Aloysius Soon, Yonsei Univ.)
Poster-7 : “Implementation and Applications of Time-accelerated Dynamics (TAD)” (Art Cho, Korea Univ.)
Poster-8 : “Recent Development of Effective Quantum-based Simulation Method” (Seungmi Lee, KRISS)
Poster-9 : “The Role of Room temperature Ionic Liquid in Electrochemical CO_2 Reduction” (Hyeongjoon Kim, KAIST)
Poster-10 : “Machine Learning Prediction of Double Perovskite Bandgaps” (Hyunju Chang, KRICT)

12:30-14:30 (Lunch & Poster)

14:30-15:00 (Invited-5) “Optimizing Materials for Solar Energy Conversion: The Roel of Defects and Interfaces”
Giulia Galli
University of Chicago, USA

15:00-15:30 (Invited-6) “Computational Synthesis and Characterization by Quantum and Reactive Molecular Dynamics”
Aiichiro Nakano
University of Southern California, USA

15:30-16:00 Break

16:00-16:30 (Invited-7) “Light Absorption of Contacted Molecules: Insights and Impediments from Atomistic Simulations”
Thomas A. Niehaus
Univ. of Lyon 1 & Institut Lumi’ere Mati’ere, France

16:30-17:00 (Invited-8) “Development of Large-scale Quantum Mechanical Molecular Dynamics Simulation: Divide-and-Conquer Density Functional Tight-binding Approach”
Yoshifumi Nishimura
Waseda University, Japan

17:00-17:30 (Invited-9) “Machine Learning Assisted Design of Polymer Dielectrics”
Chiho Kim
University of Connecticut, USA

17:30-18:00 (Wrap-up Discussion)