

FY2021 IMI Joint Usage Research Project

Perspectives on Artificial Intelligence and Machine Learning in Materials Science

2022.2/4-6
(Fri) (Sun)

Invited Speakers:

Sherry Chen (Hong Kong University of Science and Technology)
Data-driven approach for indexing-free X-ray crystallography

Xiangdong Ding (Xi'an Jiaotong University)
Artificial intelligence enhanced atomic simulations of complex phase transformation

Shigenori Fujikawa (PCNER, Kyushu University)
Membrane design for negative CO₂ emissions technology

Kulbir Kaur Ghuman (INRS)
Designing energy materials via genetic algorithm based machine learning approach

Gergely Juhasz (Tokyo Institute of Technology)
Electrochemistry of nanoparticles and nanotubes

Yu Kaneko (DAICEL Co.)
Introduction of machine learning approach for chemical compound search in Daicel

Yoshinobu Kawahara (IMI, Kyushu University and RIKEN)
Data-driven analysis of dynamical systems: from an operator-theoretic perspective

Ipppei Obayashi (RIKEN)
3D data analysis of X-ray CT images with persistent homology and nonnegative matrix factorization

Daniel Packwood (iCeMS, Kyoto University)
Data-driven approaches for surface materials and beyond

David Rivera (Hiroshima University)
Density functional theory and machine learning description and prediction of oxygen atom chemisorption on platinum nanoparticles

Petros Sofronis (PCNER, Kyushu University and UIUC)
Mathematical challenges in linking the micro-with macro-scale behavior of materials in adverse chemomechanical environments

Ichigaku Takigawa (RIKEN and Hokkaido University)
Machine learning for molecules: lessons and challenges of data-centric chemistry

Venue: Ito Campus, Kyushu University (Lecture room/W1-C512) and Online



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<https://joint.imi.kyushu-u.ac.jp/post-2698/>
Co-organizer: Shigenori Fujikawa (PCNER, K-NETS, Kyushu University) with the MOZES,
Moonshot for Beyond Zero-Emission Society <https://mozes.jp/en/>
Principal Investigator: Daniel Packwood (Institute for Integrated Cell-Material Sciences, Kyoto University)

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Yasuhide Fukumoto (IMI, Kyushu University)
Shigenori Fujikawa (PCNER, Kyushu University)
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