JST Sakigake Materials Informatics

PRESTO
International Symposium on Materials Informatics

～Learn the Data, to Bridge the Intelligence into the Future～

データを学び、知を未来へつなぐ。

URL: https://form.jst.go.jp/enquetes/m_InternationalSympo1

Research Supervisor: Shinji Tsuneyuki, Professor, School of Science, The University of Tokyo

Invited Speakers (Overseas)

Leroy Cronin, University of Glasgow (UK): “Exploring chemical reactivity with artificial intelligence & robotics”

Luca M. Ghiringhelli, Fritz-Haber Institute of the Max Planck Society (Germany):
“Topics in data-driven materials science: crowd sourcing and maps of material properties”

M. L. Green, National Institute of Standards and Technology (USA):
“AI-driven, autonomous, high-throughput materials science”

Jürg Hutter, University of Zurich (Switzerland): “MARVEL: computational design and discovery of novel materials”

Sergei V Kalinin, Oak Ridge National Laboratory (USA):
“Deep learning in scanning transmission electron microscopy: from physics to atomic manipulation”

O. Anatole von Lilienfeld, University of Basel (Switzerland): “Quantum machine learning”

Ziqin Rong, Lawrence Berkeley National Lab (USA):
“Predicative materials synthesis through machine learning and natural language processing ”

Semion K. Saikin, Kebotix, Inc. (USA): “Towards discovery of organic molecules using smart automation”

Kristof T. Schütt, Technical University of Berlin (Germany):
“SchNet - a deep learning architecture for molecules and materials”

Matthew Tucker, Oak Ridge National Laboratory (USA): “RMCProfile: moving closer to complex modelling”

Mark P. Waller, Shanghai University (PR China):
“Deep learning and discipline scale data for accelerating molecular discovery”

Logan Ward, University of Chicago (USA):
“ Combining high-throughput experimentation and machine learning”

Andrew White, University of Rochester (USA):
“Computational design of peptide-based materials with maximum entropy molecular simulation and data-driven modeling”

Hui Zhai, Tsinghua University (PR China): “Machine learning and quantum physics”

Oral Presentations from Japan by JST PRESTO, CREST & NIMS MI²I members: 14

We also have 45 poster presentations

February 9 – 11, 2019, Tokyo, Japan

Venue: Koshiba Hall, Hongo Campus, The University of Tokyo

PRESTO sakigake

JST Japan Science and Technology Agency

Strategic Basic Research Programs

http://www.jst.go.jp/kisoken/en/

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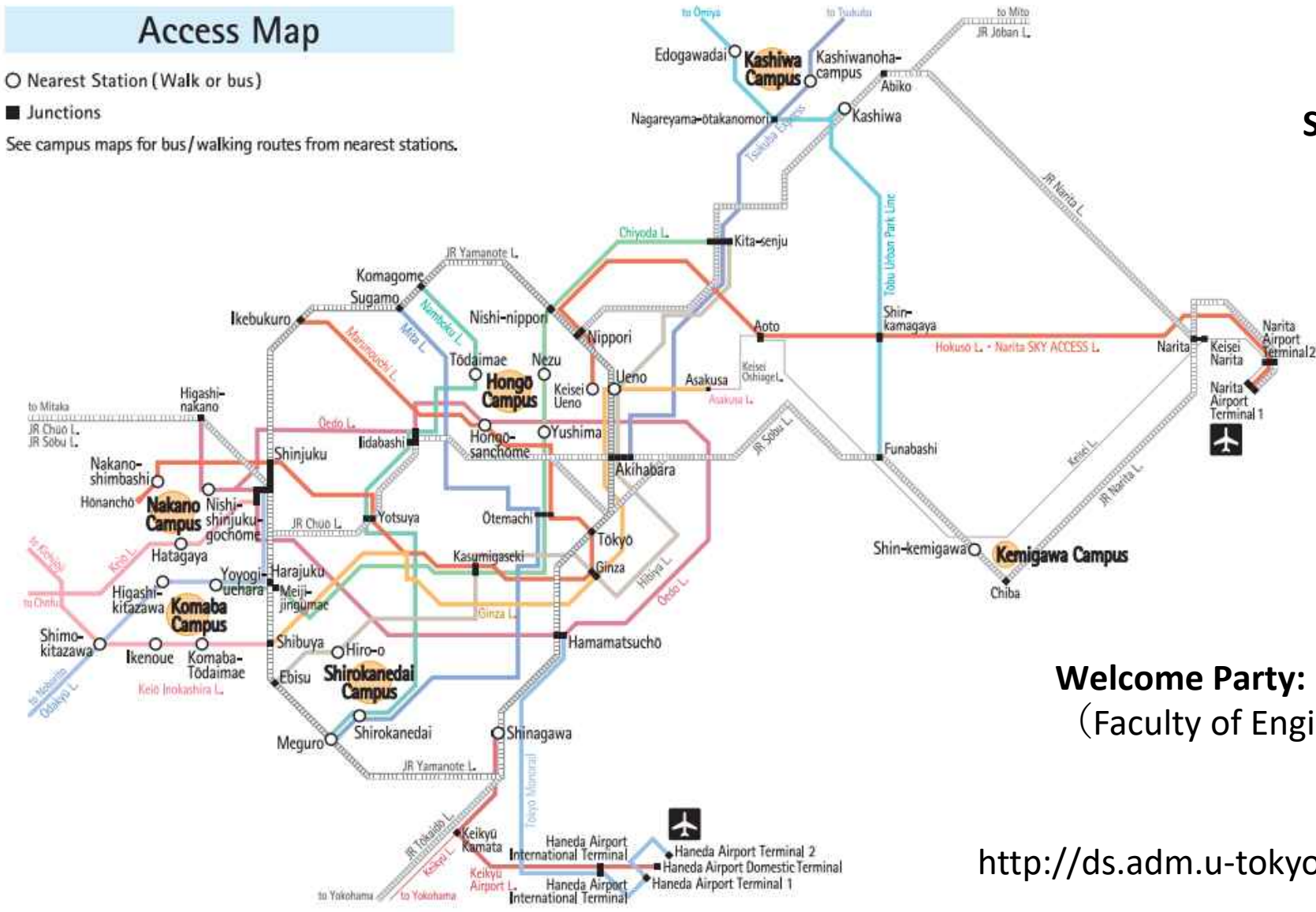
2018.12.14

JST International Symposium on Materials Informatics, February 9 – 11, 2019, Koshiba Hall, the University of Tokyo, Japan

Venue Overview

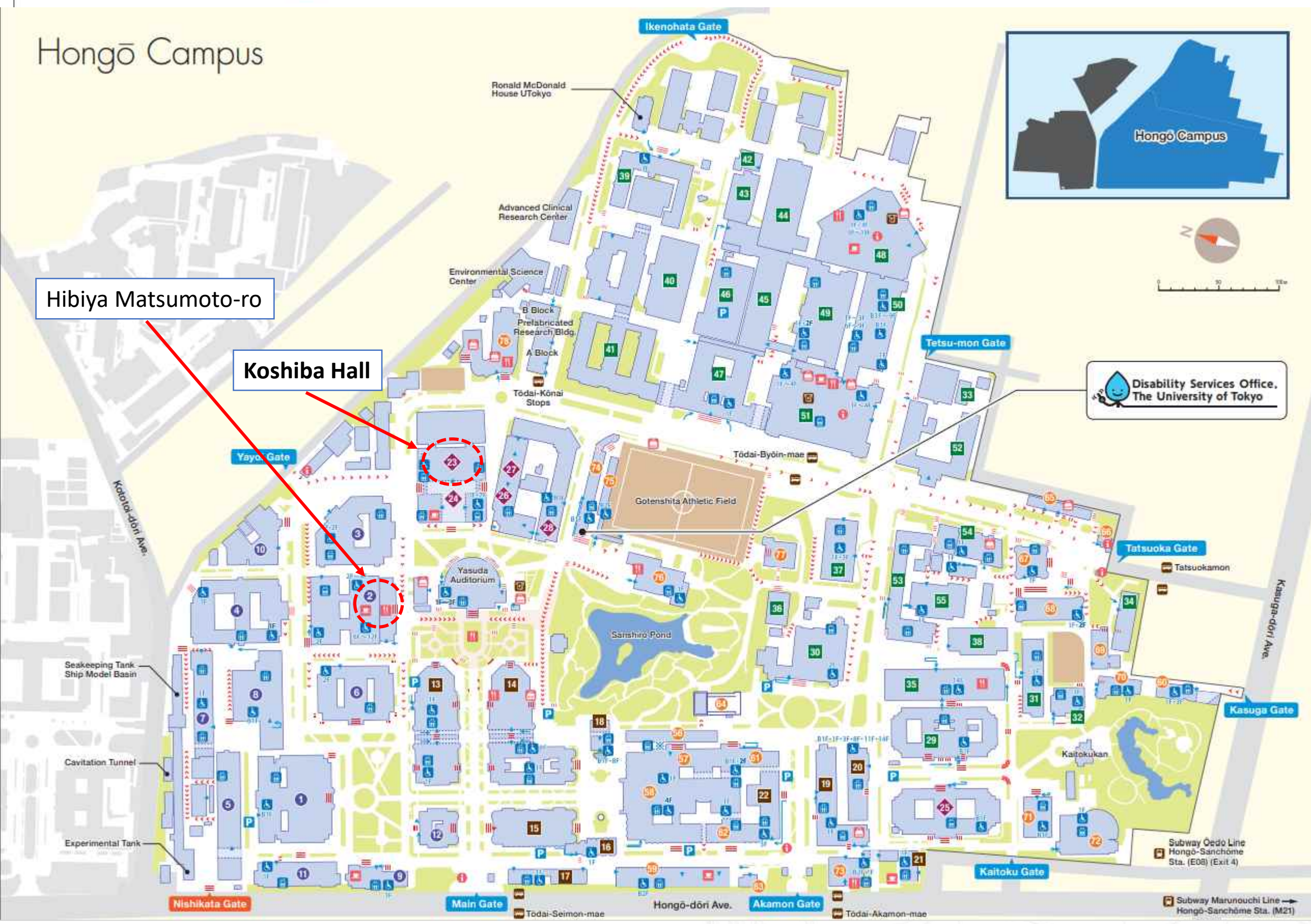
JST Sakigake Materials Informatics



Symposium: Koshiba Hall
Faculty of Science Bldg.1 (Center)
Hongo Campus, The University of Tokyo
7-3-1, Hongo, Bunkyo-ku, Tokyo, Japan

Welcome Party: Hibiya Matsumoto-ro
（Faculty of Engineering Bldg.2, The University of Tokyo）

http://ds.adm.u-tokyo.ac.jp/material/pdf/20171017104923.pdf



JST International Symposium on Materials Informatics, February 9 – 11, 2019, Koshiba Hall, the University of Tokyo, Japan

Symposium Program

JST Sakigake Materials Informatics

Oral Presentation : February 9 , Saturday, 2019 The first Day

13:00 - 13:10 [Opening Remarks] Shinji Tsuneyuki, PRESTO Research Supervisor, The University of Tokyo

13:10 - 14:40 [Session 1]

AI-driven, autonomous, high-throughput materials science
Martin Laurence Green, National Institute of Standards and Technology

Machine learning and ultrafast experimental screening of polymer and perovskite solar cells
Akinori Saeki, Osaka University / PRESTO Member : year started 2015

Machine-learning-assisted discovery of high thermal conductivity polymers using a molecular design algorithm
Junko Morikawa, Tokyo Institute of Technology

Break

14:55 - 16:35 [Session 2]

Deep learning in scanning transmission electron microscopy: from physics to atomic manipulation
Sergei V Kalinin, Oak Ridge National Laboratory

Data-driven approach for interface and spectrum
Teruyasu Mizoguchi, The University of Tokyo / PRESTO Member : year started 2016

Computational design of peptide-based materials with maximum entropy molecular simulation and data-driven modeling
Andrew White, University of Rochester

Break

16:50 - 18:10 [Session 3]

Combining high-throughput experimentation and machine learning
Logan Ward, University of Chicago

Machine learning interatomic potential with group-theoretical high-order rotational invariants
Atsuto Seko, Kyoto University / PRESTO Member : year started 2015

Liquid electrolyte materials search for li-ion batteries
Keitaro Sodeyama, National Institute for Materials Science (NIMS) / PRESTO Member: year started 2015

18:30 – 20:30 [Welcome Party] Hibiya Matsumoto-ro at Faculty of Engineering Bldg.2

JST International Symposium on Materials Informatics, February 9 – 11, 2019, Koshiba Hall, the University of Tokyo, Japan

Symposium Program

JST Sakigake Materials Informatics

Oral Presentation : February 10 , Sunday, 2019 The second Day

9:30 - 11:00 [Session 4]

MARVEL: computational design and discovery of novel materials
Jürg Hutter, University of Zurich

Computational design and exploration of novel semiconductors
Fumiyasu Oba, Tokyo Institute of Technology / National Institute for Materials Science / JST CREST [Revolutional Materials Development] Research Director : year started 2016

Machine learning and surrogate optimization on heterogeneous catalysts
Ichigaku Takigawa, Hokkaido University / PRESTO Member : year started 2015

Break

11:20 - 12:20 [Session 5]

Exploring chemical reactivity with artificial intelligence & robotics
Leroy Cronin, University of Glasgow

Material development by explainable machine learning
Yuma Iwasaki, NEC Corporation / PRESTO Member : year started 2017

12:20 - 14:30 [Lunch and Poster Session1]

14:30 - 16:10 [Session 6]

Towards discovery of organic molecules using smart automation
Semion K. Saikin, Kebotix, Inc.

Database and machine-learning enabled new insights into the lanthanide luminescent materials
Miho Hatanaka, Nara Institute of Science and Technology / PRESTO Member : year started 2015

Quantum machine learning
O. Anatole von Lilienfeld, University of Basel

Break

16:30 - 17:30 [Session 7]

RMCProfile: moving closer to complex modelling
Matthew Tucker, Oak Ridge National Laboratory

Parameter estimation from microstructure evolution by phase-field method and adjoint method
Yuhki Tsukada, Nagoya University / PRESTO Member : year started 2015

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Symposium Program

JST Sakigake Materials Informatics

Oral Presentation : February 11 , Monday, 2019 The third Day

9:30 - 11:20 [Session 8]

Topics in data-driven materials science: crowd sourcing and maps of material properties
Luca M. Ghiringhelli, Fritz-Haber Institute of the Max Planck Society

Efficient ab initio prediction of thermal properties of solids assisted by machine learning
Terumasa Tadano, National Institute for Materials Science (NIMS)

Deep learning and discipline scale data for accelerating molecular discovery
Mark P. Waller, Shanghai University

Break

11:40 - 12:40 [Session 9]

Mining magnetic materials data
Dam HieuChi , Japan Advanced Institute of Science and Technology(JAIST) / PRESTO Member : year started 2015

Predicative materials synthesis through machine learning and natural language processing
Ziqin Rong, Lawrence Berkeley National Lab

12:40 - 13:40 [Lunch and Poster Session2]

13:40 - 15:40 [Session 10]

SchNet - a deep learning architecture for molecules and materials
Kristof T. Schütt, Technical University of Berlin

Statistical machine learning for spectrum image data analysis
Motoki Shiga, Gifu University / PRESTO Member : year started 2016

Machine learning and quantum physics
Hui Zhai, Tsinghua University

Hidden mechanism of high-temperature superconductivity revealed by solving non-linear inverse problems
Yohei Yamaji, The University of Tokyo / PRESTO Member : year started 2015

15:40 - 16:00 [Closing]

Symposium Program

JST Sakigake Materials Informatics

Poster Presentation : February 10, 12:30 - 14:30 / February 11 , 12:30 - 13:30 PRESTO

Precursory Research for Embryonic Science and Technology : PRESTO

PRESTO Members: Year Started 2015

Development of unexplored materials promoted by first-principles calculation and informatics
Isao Ohkubo, National Institute for Materials Science (NIMS)

Machine learning based efficient exploration of crystal interface structures
Masayuki Karasuyama, Nagoya Institute of Technology

Studies on metal nanocluster catalyst with informatics and automated reaction path search
Masato Kobayashi, Hokkaido University

Unravelling diffraction from glass, liquid, and amorphous materials
Shinji Kohara, National Institute for Materials Science (NIMS)

Systematic generation of tight-binding Hamiltonian for ferromagnets and its application
Takashi Koretsune, Tohoku University

Correctness judgment of reconstruction by compressive sensing on discrete tomography
Chihiro Nakajima, PRESTO researcher, Japan Science and Technology Agency

Topological data analysis for the molecular dynamics simulation
Takenobu Nakamura, National Institute of Advanced Industrial Science and Technology

PRESTO Members: Year Started 2016

Machine learning approach for the analysis of X-ray absorption spectra
Hidekazu Ikeno, Osaka Prefecture University

Materials-informatics-assisted high-yield synthesis of nanosheets through exfoliation
Yuya Oaki, Keio University

Speed up of quantum dot sensors utilizing Bayesian estimation
Tomohiro Otsuka, Tohoku University

Machine learning of oxygen vacancy formation energies
Yu Kumagai, Tokyo Institute of Technology

Self-learning continuous-time quantum Monte Carlo and optimization of the single-particle basis
Naoto Tsuji, RIKEN

Symposium Program

JST Sakigake Materials Informatics

Poster Presentation : February 10, 12:30 - 14:30 / February 11 , 12:30 - 13:30 PRESTO

A systematic exploration of conical intersections based on time dependent density functional theory: toward a theoretical screening of photo-functional molecules
Yu Harabuchi, Hokkaido University

Informatics techniques and descriptors for finding novel solid electrolyte candidates by computational screening
Jalem Randy, National Institute for Materials Science (NIMS)

Efficient molecular structure search based on Bayesian inference
Kenta Hongo, Japan Advanced Institute of Science and Technology (JAIST)

Exploring azeotropic binary mixtures for green cooling
Hirotoshi Mori, Ochanomizu University

PRESTO Members: Year Started 2017

Modulating photo- and electroluminescence of a stimuli-responsive π-conjugated molecule
Naoya Aizawa, PRESTO Researcher, Japan Science and Technology Agency

Sparse modeling of EXAFS
Yukihiko Igarashi, PRESTO Researcher, Japan Science and Technology Agency

Mathematical structures behind grain-boundary atomic arrangements and atomic-scale observations
Kazutoshi Inoue, PRESTO Researcher, Japan Science and Technology Agency

Structural-controlled synthesis of single-walled carbon nanotubes based on machine-learning approach
Toshiaki Kato, Tohoku University

Creation of novel functionalities in metal hydrides thin films using fully-automatic and autonomous growth processes
Ryota Shimizu, Tokyo Institute of Technology

Development of material search methods in lithium ion conducting oxides using machine learning
Kota Suzuki, Tokyo Institute of Technology

First-principles prediction of magnetic structures in crystal
Michito Suzuki, Tohoku University

Symposium Program

JST Sakigake Materials Informatics

Poster Presentation : February 10, 12:30 - 14:30 / February 11 , 12:30 - 13:30 PRESTO

Orbital-free density functional theory with semi-local machine-learned kinetic energy density functional

Junji Seino, Waseda University

Elucidation of the crystalization process of pillared-layer metal-organic frameworks using microreactors

Daisuke Tanaka, Kwansei Gakuin University

High-throughput peak shift detection using machine learning for synchrotron X-ray spectral imaging

Naoka Nagamura, National Institute for Materials Science (NIMS)

Material Informatics for designs of biomaterials

Tomohiro Hayashi, Tokyo Institute of Technology

Similarity between synthesis conditions by tensor factorization of synthesis database

Hiroyuki Hayashi, Kyoto University

Determination of quantum chemistry wave function using artificial neural network based quantum state model

Takeshi Yanai, Nagoya University

JST CREST [Revolutional Materials Development] : year started 2018

Design and development of organic semiconductors: toward using materials informatics

Tatsuo Hasegawa, The University of Tokyo / CREST Research Director

Symposium Program

JST Sakigake Materials Informatics

Poster Presentation : February 10, 12:30 - 14:30 / February 11 , 12:30 - 13:30 NIMS MI²I

National Institute for Materials Science (NIMS) "Materials research by Information Integration" Initiative (MI²I)

Quantitative estimation of importance of descriptors on curie temperatures of rare-earth transition metal binary systems based on subgroup relevance analysis
Hiori Kino

Starrydata: a plot mining web system for experimental materials informatics
Yukari Katsura, The university of Tokyo

Development of crystal structure prediction tool
Tomoki Yamashita, Osaka University

Synergic collaboration of quantum beam measurements, modelling, and mathematics to unravel liquid matter: towards a collaboration with microgravity in space
Yohei Onodera, Kyoto University

Topological analysis of magnetic domain structures based on persistent homology
Masato Kotsugi, Tokyo University of Science

Transfer learning: a next key driver of accelerating materials discovery with machine learning
Chang Liu, The Institute of Statistical Mathematics

Bayesian inference for molecular design and retro-synthesis
Guo Zhongliang, The Graduate University for Advanced Studies

Development of linearly independent descriptor generation method for empirical law discovery
H. Fujii, Osaka Universiry

Analysis of grain boundary structure using persistent homology
Fumiko Ogushi, Kyoto University

Sparse modeling for elucidating physical mechanisms
Tamio Oguchi, Osaka University

Symposium Program

JST Sakigake Materials Informatics

Poster Presentation : February 10, 12:30 - 14:30 / February 11 , 12:30 - 13:30 NIMS MI²I

Forward and backward prediction of crystal growth simulation using machine learning
Yukinori Koyama

Development of ultra low thermal conductivity nano-composite by interface design
Yibin Xu and Yen-Ju Wu

Data-driven materials exploration for li-ion conductive ceramics by exhaustive and Informatics-aided computations
Robyn E. Ward and Masanobu Nakayama, Nagoya Institute of Technology

Thermophysical property database of solids for materials informatics
Tetsuya Baba

Surface/Interface roughness optimization for thermal transport using Monte Carlo tree search
T. Dieb, The University of Tokyo

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STRATEGIC BASIC RESEARCH PROGRAMS

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