2021年度共同利用研究報告書

2022年04月21日

所属・職名 Institute for Integrated Cell-Material Sciences, Kyoto University・Junior Associate Professor

Daniel PACKWOOD

		整理番号	20210014	
1.研究計画題目	Perspectives on Artificial Intelligence and Machine Learning in Materials Science			
2.新規・継続	新規			
3.種別	一般研究			
4.種目	研究集会(I)			
5.研究代表者	氏名	Daniel PACKWOOD		
	所属 部局名	Institute for Integrated Cell-Material Sciences, Kyoto University	職名	Junior Associate Professor
6.研究実施期間	2022年02月04日(金曜日)～2022年02月06日(日曜日)			
7.キーワード	Materials science, Artificial Intelligence, machine learning, non—linear dynamics, persistent homology, evolutionary algorithms, global optimization algorithms, accelerated discovery of metal alloys, soft materials, complex oxides, density functional theory, Bayesian methods, dynamical systems [PDEs and ODEs], stochastic methods [Monte Carlo]			
8.参加者人数	50人			

9.本研究で得られた成果の概要

The purpose of this conference was to gather an international group of researchers in industry and academia bringing their own distinct perspectives on problems at the intersection of Materials Physics and Information Technology, two areas where interdisciplinary collaborations both at the academic and industrial level are crucial and yet to date in early phase.

The conference was held on-line over 3 days and saw participation of approximately 50 participants including from North America and China.

The conference was organized as an IMI joint usage Research Seminar 1 and co-sponsored by the MOZES program. The conference consisted of 12 invited lectures and a students' session with 11 students' talks.

We expect significant new collaborations will emerge as a result of this conference, in particular, across IMI/I2CNER and Xi'an Jiaotong and UIUC/Montreal, among others.

Report of: Perspectives on Artificial Intelligence and Machine Learning in Materials Science, February 4-6, 2022

Artificial Intelligence has led to a paradigm shift in investigation in Materials Science, with Machine Learning allowing informatics-based systematic calculations, predictions and discovery based on material databases pushing beyond the intrinsic limitations of first-principles calculations. However, the successful application requires development of novel methodologies inspired by the frontends of materials development in close synergy between physical science and Information Technology.

For example, demand is growing for functional molecules capable of performing specific work cycles such as assembly and transportation of molecules, cyclization and cycloreversion. These specific functionalities require the design and customization of molecular architectures at the atomistic level. This is a task which requires quantum chemistry modeling (so that chemical and physical properties are computed as the result of the atomic composition of the architecture) and inverse design (so that the atomic composition→ property mapping can be effectively inverted). Nowadays, complex numerical platforms blending first-principle computations, genetic algorithms for the exploration of high-dimensional chemical spaces, machine learning models for regression and classification over large pools of molecules and bioinformatics techniques for the digitalization and codification of molecular formulas have been largely exploited for the discovery of dielectric materials, perovskites, nanoparticles and more. However, outstanding questions remain unexplored, such as the coordination of nano- and meso- scale optimization programs, the identification of effective molecular descriptors capable of passing on relevant information to train machine learning models, the definition of suitable surrogate models and optimization strategies and many more.

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Despite the conference was held in on-line version, the 3 days were rich in discussions and saw the participation of approximately 50 participants including from North America and China. Among topics covered were the exploitation of supervised learning techniques for high-throughput chemical calculations, regression methods to discover relations among meso-scale phenomena and nano/micro properties, genetic algorithms, materials characterization, data-driven approaches to dynamical systems, design of materials with Artificial Intelligence techniques.

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Plan for publication of the proceedings. We intend to publish IMI Lecture Notes and we will submit our draft later in June 2022.

Plan for publication of other results. Some of the participants might initiate and carry on new collaborations including joint papers in the future. We will notify all speakers to add an explicit acknowledgment to their papers resulting from collaborations initiated thanks to our conference.

Principal Investigator: Daniel PACKWOOD (Junior Associate Professor/Institute for Integrated Cell-Material Sciences, Kyoto University)

Co-organizers (Alph.)
Pierluigi Cesana, IMI Kyushu University
Shigenori Fujikawa, I^{2}CNER Kyushu University
Yasuhide Fukumoto, IMI Kyushu University
Petros Sofronis, UIUC and I^{2}CNER Kyushu University
Alex Staykov I^{2}CNER Kyushu University

10th ANNIVERSARY
Institute of Mathematics for Industry
Kyushu University

MOZES
Moonshot for
beyond Zero-Emission Society

List of students
Students talks schedule:Friday 4th

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Friday 4th

2.00-2.15 pm Jose Madrid, “Automated defects detection via Machine Learning”, INRS EMT, Canada, graduate student
2.15-2.30 pm Aghrazaei Parastoo, “Design of Cu-Ni based alloys for electrochemical ammonia production via Special Quasi-random Structures (SQS) and Genetic Algorithm”, INRS, Canada, graduate student
2.30-2.45 pm Sebastian Graiff Zurita, "Reconstruction of Log-aesthetic curve parameters", Kyushu Graduate School of Mathematics, PhD student
2.45-3.00 pm Morio Nakatani, 九州大学カーボンニュートラル・エネルギー国際研究所, Graduate student
3.00-3.15 pm Anant Vaishnav, “Investigation of confinement effect of PDMS on CO2”, 九州大学カーボンニュートラル・エネルギー国際研究所, Graduate student

Saturday 5th
2.00-2.15 pm Junzhi Zheng, “ Solutions to a new strongly coupled phase-field model for nematic liquid crystals with variable degree of orientation“, Department of Mathematics, Shanghai University, PhD student
2.15-2.30 pm Thi Nguyen Xuan, "Computational study on the oxygen diffusion mechanism in fluorite lattices", 九州大学カーボンニュートラル・エネルギー国際研究所, Graduate student
2.30-2.45 pm Debashis Sahu, MCI-CNRC in I 2CNER at Kyushu University,
postdoc
2.45-3.00 pm Takaya Fujisaki, “Density functional theory analysis for adsorption of hydrogen sulfide on graphene-based structures “ , 東北大学Tohoku University, Postdoc
3.00-3.15 pm Linh Nguyen Thi Hoai, “Title: Mineralization Process in Porous Media using Random Walk with Absorption”, 九州大学マス・フォア・インダストリ研究所, Postdoc
3.15pm-3.30pm Fuzhu Liu, “Ensemble Effect of Pd@Au Electrocatalysts on CO2 Reduction Reaction: A DFT-based Machine-learning Study”, Xi'an Jiaotong University, Postdoc

IMI Workshop of the Joint Research Projects in Kyushu University

Perspectives on Artificial Intelligence and Machine Learning in Materials Science

Date： February 4 (Fri) – 6 (Sun), 2022
Place： Lecture Room (W1-C-512), West Zone 1,
Ito campus, Kyushu University and Live streaming by Zoom
Principal Investigator：Daniel PACKWOOD (Institute for Integrated Cell-Material Sciences, Kyoto University)

February 4 (Fri), 2022 (Chair: Alex STAYKOV)

8:30-8:40
Opening Remarks (Yasuhide FUKUMOTO)

08:40-09:40
Mathematical Challenges in Linking the Micro- with Macro-Scale Behavior of Materials in Adverse Chemomechanical Environments
Petros SOFRONIS (I^2CNER, Kyushu University and UIUC)

09:40-10:40
Designing Energy Materials via Genetic Algorithm Based Machine Learning Approach
Kulbir Kaur GHUMAN (INRS)

10:40-11:00 Break

11:00-12:00
Density Functional Theory and Machine Learning Description and Prediction of Oxygen Atom Chemisorption on Platinum Nanoparticles
David RIVERA (Hiroshima University)

12:00-13:00
Electrochemistry of Nanoparticles and Nanotube
Gergely JUHASZ (Tokyo Institute of Technology)

13:00-14:00 Lunch Break

14:00-16:00 Student talks session

February 5 (Sat), 2022 (Chair: Daniel PACKWOOD)

08:30-09:30
Membrane Design for Negative CO2 Emissions Technology
Shigenori FUJIKAWA (I^2CNER, Kyushu University)

09:30-10:30
Introduction of Machine Learning Approach for Chemical Compound Search in Daicel
Yu KANEKO (Daicel Corporation)

10:30-11:00 Break

11:00-12:00
Machine Learning for Molecules: Lessons and Challenges of Data-Centric Chemistry
Ichigaku TAKIGAWA (RIKEN and Hokkaido University)

12:00-13:00
3D Data Analysis of X-Ray CT Images with Persistent Homology and Nonnegative Matrix Factorization
Ippei OBAYASHI (RIKEN）

13:00-14:00 Lunch Break

14:00-16:00
Student talks session

February 6 (Sun), 2022 (Chair: Pierluigi CESANA)

08:30-09:30
Data-Driven Approaches for Surface Materials and Beyond
Daniel PACKWOOD (iCeMS, Kyoto University)

09:30-10:30
Data-Driven Analysis of Dynamical Systems: From an Operator-Theoretic Perspective
Yoshinobu KAWAHARA (IMI, Kyushu University and RIKEN)

10:30-11:00 Break

11:00-12:00
Data-Driven Approach for Indexing Free X-Ray Crystallography
Sherry CHEN (Hong Kong University of Science and Technology)

12:00-13:00
Artificial Intelligence Enhanced Atomic Simulations of Complex Phase Transformation
Xiangdong DING (Xi'an Jiaotong University)

13:00-13:10
Closing remarks

13:10-14:00 Lunch Break

14:00-16:00
Room breakout/free discussions/Student talks session