FY2025 Grant for International Project Research IMI Joint Use Research Program Proposal

2025/01/28

所属・職名 INRS (Montreal, Canada)・Associate Professor

Name: Kulbir Ghuman

		整理番号	2025b007	
1.研究計画題目	Advancing Materials Data, Design, and Discovery			
2.新規・継続	Continued			
3.種別	国際プロジェクト研究			
4.種目	研究集会（Ｉ）			
5.開催方法				
6.研究代表者	氏名	Kulbir Ghuman		
	所属部局名	INRS (Montreal, Canada)	職名	Associate Professor
7.研究実施期間	2025年04月23日～2025年04月25日			
8.キーワード	Materials Science, Artificial Intelligence, Machine Learning, Orbital-Free Density Functional Theory, Molecular Dynamics, Optimal Transport, global optimization algorithms, accelerated discovery of metal alloys, complex oxydes.			
9.参加者人数	59			

10.本研究で得られた成果の概要

Summary of the 3rd CEMDI-PAIMS Symposium

Title: Advancing Materials Data, Design, & Discovery

Date: April 23–25, 2025

Venue: I2CNER Hall C, Kyushu University, Japan

The 3rd CEMDI-PAIMS Symposium brought together 60 participants from Japan, Canada, and beyond to explore the intersection of Artificial Intelligence (AI), computational modeling, and materials science. Co-hosted by Kyushu University's I2CNER and IMI, the symposium continued efforts to accelerate materials discovery through data-driven approaches.

The event opened with institutional overviews from I2CNER, IMI, and Canada's PRIMA, setting the stage for a series of technical sessions. Presentations covered a range of topics including machine learning-assisted design of porous materials, orbital-free DFT, multiscale modeling, and optimal transport methods. Talks also addressed CO_2 capture, solid-state electrolytes, and the application of AI to high-entropy alloys and functional molecules.

The program featured four major themes:

1.AI for Materials Discovery

2.Computational Chemistry and Physics

3.Modeling for Electrochemical and Energy Devices

4.Experimental-Computational Integration

A dedicated session on Quebec–Japan collaboration highlighted institutional support from PRIMA and the Québec Delegation in Tokyo. The symposium concluded with oral presentation awards and lab tours. This event marked the fourth in the growing CEMDI-PAIMS series. Organizers confirmed plans to continue this international collaboration, alternating between Canadian and Japanese host institutions, with a strong emphasis on student training, research exchange, and joint projects. IMI funding has helped strengthen the QC–Japan collaboration, leading to a jointly organized event scheduled to take place in Montreal next year. Additionally, efforts are currently underway with delegates from both Québec and Japan, as well as Québec funding agencies, to initiate an official partnership.

Summary of the 3rd CEMDI-PAIMS Symposium
Title: *Advancing Materials Data, Design, & Discovery*
Date: April 23–25, 2025
Venue: I2CNER Hall C, Kyushu University, Japan
The 3rd CEMDI-PAIMS Symposium brought together 60 participants from Japan, Canada, and beyond to explore the intersection of Artificial Intelligence (AI), computational modeling, and materials science. Co-hosted by Kyushu University's I2CNER and IMI, the symposium continued efforts to accelerate materials discovery through data-driven approaches.
The event opened with institutional overviews from I2CNER, IMI, and Canada's PRIMA, setting the stage for a series of technical sessions. Presentations covered a range of topics including machine learning-assisted design of porous materials, orbital-free DFT, multiscale modeling, and optimal transport methods. Talks also addressed CO_2 capture, solid-state electrolytes, and the application of AI to high-entropy alloys and functional molecules.
The program featured four major themes:

1. **AI for Materials Discovery**
2. **Computational Chemistry and Physics**
3. **Modeling for Electrochemical and Energy Devices**
4. **Experimental-Computational Integration**

A dedicated session on Quebec–Japan collaboration highlighted institutional support from PRIMA and the Québec Delegation in Tokyo. The symposium concluded with oral presentation awards and lab tours. This event marked the fourth in the growing CEMDI-PAIMS series. Organizers confirmed plans to continue this international collaboration, alternating between Canadian and Japanese host institutions, with a strong emphasis on student training, research exchange, and joint projects. IMI funding has helped strengthen the QC–Japan collaboration, leading to a jointly organized event scheduled to take place in Montreal next year. Additionally, efforts are currently underway with delegates from both Québec and Japan, as well as Québec funding agencies, to initiate an official partnership.

1. Motivation for the Research Plan

The **"Advancing Materials Data, Design, and Discovery" International Research-Workshop (I)** was created to address the need to bring together different scientific fields — especially **materials science, chemistry, and mathematical modeling** — with a strong focus on **applied statistics** and **artificial intelligence**. Although AI — and in particular, **machine learning (ML)** — has already made major impacts in many areas of science, using AI in **materials science** comes with special challenges. Traditional computational methods like **Density Functional Theory (DFT)** require a lot of computing power and often struggle to handle large or complex systems. By combining AI with these traditional methods, researchers can speed up how new materials are predicted, designed, and discovered. But to truly achieve this, new ways of connecting materials science with AI, mathematical modeling, and data science informatics need to be developed.

The workshop brought together about **60 participants**, including university professors, graduate students, industry experts, and leaders from institutions in **Canada and Japan**. This diverse group explored the latest developments in using AI to solve materials science problems. Key topics included **orbital-free DFT**, **multiscale modeling**, and **optimal transport-based learning** — all of which represent new and promising directions in computational materials research.

Another important topic of discussion was the **quality of data** currently used in materials science. Many participants emphasized the need to improve **data infrastructure** — especially to make materials data more complete, accurate, and easier to use. This is essential for AI tools to work effectively in predicting and designing materials.

Overall, the event provided an important opportunity for **knowledge sharing** and building **stronger connections** among experts in different fields — including computational chemistry, materials science, AI, and mathematics. These collaborations will be vital for the future of materials discovery and design.

2. Continuation and Future Development of the Project

The 2025 symposium was the fourth edition of the PAIMS series, which began in 2022 as part of the CEMDI-PAIMS initiative. The first events were held online due to the COVID-19 pandemic, but the series quickly grew into an international platform for research collaboration. Past symposia were hosted by Waseda University (2023) and INRS Montréal (2024). Each year, the event has expanded in size and participation, with a special focus on building stronger ties between Japan and Canada. The 2025 symposium continued this effort, especially by working to strengthen partnerships between leading institutions from both countries.

A key goal of the 2025 event was to make existing collaborations more formal and build new ones — especially with organizations like PRIMA (Quebec's Advanced Materials Research and Innovation Hub). These partnerships aim to support new research projects, student exchange programs, and joint applications for research funding. PRIMA is a strong partner because it connects Quebec's academic world with industry. During the symposium, special meetings were held between Dr. Rusoma Akilimali (Technology and Innovation Advisor at PRIMA) and leading researchers from IMI to explore common research interests.

Importantly, discussions have already started on student exchanges between Japanese and Canadian laboratories at different levels. The symposium helped make these conversations possible and encouraged networking that could lead to future collaborations. One clear result is a joint research paper now being prepared for submission, which will acknowledge support from the International Research-Workshop (I).

Looking ahead, the CEMDI-PAIMS initiative will continue as a regular event. It will provide a space for expanding collaboration between universities and industries, and for strengthening international ties between Japan and Canada. The 2025 symposium played an important role in supporting these goals, and discussions are already happening about the next editions. The plan is to rotate hosting between Japanese and Canadian institutions to keep up the momentum and increase the event's global reach.

This international approach will help promote dialogue across borders, support the use of AI in materials science, and build a strong global research network.
In conclusion, the 2025 symposium was both a major achievement for the CEMDI-PAIMS series and a key step toward the future of Japan–Canada collaboration in AI-driven materials science.

開催日：2025/04/23〜2025/04/25

Advancing Materials Data, Design, and Discovery｜2025b007

カテゴリー：イベント　タグ：国際研究　研究集会I

開催概要

- **開催方法**：対面開催
- **開催場所**：九州大学 伊都キャンパス I2CNER HallC
- **主要言語**：英語
- **共催**：International Institute of Carbon Neutral Energy Research (I2CNER), (IMI)
- **種別・種目**：国際プロジェクト研究-研究集会（Ⅰ）
- **研究計画題目**：Advancing Materials Data, Design, and Discovery｜2025b007
- **研究代表者**：Kulbir Ghuman (INRS (Montreal, Canada)・Associate Professor)
- **研究実施期間**：2025年4月23日 (水) - 2025年4月25日 (金)
- **公開期間**：2025年4月23日 (水) - 2025年4月25日 (金)
- **研究計画詳細**：https://joint2.imi.kyushu-u.ac.jp/en_research_chooses/view/2025b007

プログラム

https://cemdi.inrs.ca/2025symposium

4月23日

Session I: Opening Remarks
Chair: Aleksandar Staykov

9:30

Tatsumi Ishihara (Director, I2CNER,Kyushu University, Japan)

Introduction to International Institute for Carbon-Neutral Energy Research(I2CNER)

9:40

Kenji Kajiwara (Director, IMI,Kyushu University,Japan)

Introduction to Institute of Mathematics
for Industry (IMI)

9:50

Rusoma Akilimali (Technology and Innovation Advisor,
PRIMA, QC, Canada)

Promoting Québec-Japan Collaboration
in Advanced Materials

10:00

Fiorenzo Vetrone (Professor and UNESCO Chair, INRS,
Université du Québec, Canada)

Introduction to Institut National de la Recherche Scientifique and Goals of UNESCO Chair in Materials and Technologies for Energy Conversion,Saving and Storage

10:10

Kulbir Ghuman (Director CEMDI and
Associate Professor,INRS, Université du Québec, Canada PAIMS)

Computational Energy Materials Design
Infrastructure (CEMDI): Goals and Opportunities)

10:20

Aleksandar Staykov (Associate Professor,
I2CNER)

Perspective of Artificial Intelligence in
Materials Science (PAIMS)

10:30-10:40 COFFEE BREAK

Session II: AI for Materials Discovery
Chair: Pierluigi Cesana

10:40

Xiangdong Ding (Professor and Dean,School of Materials
Science andEngineering, Xi'an Jiaotong University
Deputy Director,State Key Laboratory for Strength and
Technology of Materials)

Self-supervised probabilistic models for exploring shape memory alloys

11:10

Tom Woo (Professor, University of Ottawa, ON, Canada)

Machine learning Assisted Design of Porous Materials for CO2 capture using Integrated Atomistic Scale and Process Scale simulations

11:40

Daniel Packwood (Associate Professor, Institute for Integrated Cell-Material Sciences (iCeMS), Kyoto University, Japan)

Machine learning for functional molecular materials and supramolecular assemblies

12:10-13:10 Lunch

Session III: AI for Materials Discovery
Chair: Tsuneyuki Ozaki

13:10

Adroit Fajar (Assistant Professor, I2CNER,Kyushu University,Japan)

Can AI Truly Revolutionize Molecular Design?

13:40

Adrian Xiao Bin Yong (Postdoctoral Fellow,
I2CNER CESD,Kyushu University,Japan)

Dismai-Bench: Benchmarking generative
models using disordered materials

14:10

El Tayeb Bentria (Researcher,Qatar Environment and
Energy Research Institute, HBKU)

Computational Materials Science in the Era of Large Language Models:Challenges and Opportunities

14:40

Chandra Veer Singh (Professor,University of Toronto, Canada)

AI-enabled discovery of high-entropy materials for electrochemical energy conversion and storage

15:10-15:20 COFFEE BREAK

Session IV: Computational Modelling for Electrochemical Devices
Chair: David S. R. Rocabado

15:20

Jose C. M. Madrid (Postdoctoral Fellow, INRS,Université du Québec, Canada)

Aluminium and Iron Impurity Segregation in Yttria-Stabilized Zirconia Grain Boundaries

15:50

Takaya Fujisaki (Assistant Professor, Faculty
of materials for energy, Shimane University, Japan)

Optimizing Graphene Defects for Enhanced H_2S Adsorption in Solid Oxide Fuel Cells-A First-Principles Investigation

16:20

Alex Hernandez-Garcia (Assistant Professor, Mila, Université de Montréal, Canada)

A Curated Dataset of Crystal Structures and Experimentally Measured Ionic Conductivities for Lithium Solid-State Electrolytes

16:50

Tsuneyuki Ozaki (Professor, INRS-EMT, Canada)

Intense terahertz field-induced impact ionization in narrow bandgap semiconductors

17:20 CLOSING

4月24日

Session I: Computational Chemistry for Material Design
Chair: Chandra V. Singh

9:30

Gilles Peslherbe (Professor, Concordia University, QC, Canada)

Multiscale Modeling and Design of Electrocatalysts for the Paradigm Nitrogen Reduction Reaction: from Data-Driven High Throughput Screening to DFT Accounting for Electrode Potential Atomistic Details

10:00

Juan Shang (Assistant Professor, I2CNER, Kyushu University, Japan)

Applications of DFT calculations in theoretical design of photocatalyst and elucidation of materials degradation mechanism

10:30

Daniel Gueckelhorn (PhD student,INRS, Université du Québec, Canada)

Density functional theory study of electrical properties of misfit dislocations in SrTiO3

10:50-11:00 COFFEE BREAK

Session II: AI for Materials Discovery
Chair: Sergei Manzhos

11:00

Kazuki Yoshizoe (Professor, Research Institute for Information Technology, Kyushu University, Japan)

Accelerating Molecular Discovery with Game AI methods and Supercomputers

11:30

Shivam Dangwal (PhD Student,WPI-I2CNER, Department of Automotive Science, Kyushu University, Japan)

Towards prediction of formation enthalpy of high-entropy alloys for hydrogen storage: Machine learning, density functional theory and experimental approaches

11:50

Junji Hyodo (Associate Professor,Center for Energy System Design (CESD), I2CNER,Kyushu University,Japan)

Accelerated discovery of novel proton-conducting ceramics utilizing experimental data and machine learning

12:20-13:20 Lunch

Session III: Modeling and Calculations: From Atomic Structure to Applications
Chair: Edoardo Fabbrini

13:20

Alfio Grillo (Professor, Politecnico di Torino,Italy)

Combining asymptotic homogenization and strain-gradient inelasticity for determining the effective coefficients of a multi-layered, elasto-plastic biological material

13:50

Shunsuke Kobayashi (Assistant Professor, Osaka University, JP)

Dislocation and disclination in crystalline materials: a differential geometryapproach

14:20

Fiorenzo Vetrone (Professor, INRS,Université du Québec, Canada)

Frontiers in Rare Earth Doped Nanoparticles: Design, Properties, and Applications

14:50-15:00 COFFEE BREAK

Session IV: Accelerating Materials Discovery: New Approaches and methods
Chair: Daniel Packwood

15:00

Linh Thi Hoai Nguyen (Assistant Professor, I2CNER, Kyushu University, Japan)

Accelerating Material Discovery through an Automated and Data-Driven Workflow

15:30

Natsuhiko Yoshinaga (Professor,Department of Complex and Intelligent Systems, Future University, Hakodate, Japan)

Reinforcement learning for self-assembly problems

16:00

Antoine Diez (Postdoctoral Fellow,Kyoto University, Japan)

Multicellular simulations with shape and volume constraints using optimal transport

16:30

Ettore Barbieri (Senior Researcher, JAMSTEC, Japan)

Algorithms for Aggregation, Percolation, and Thermoelasticity in Pyroresistivity of Conductive Polymer Composites

17:00

CLOSING

4月25日

Session I: Experimental Materials Science Supported by Computational Analysis
Chair: Paul O'Brien

9:30

Jacqueline Hidalgo-Jiménez (PhD student, Graduate School of Integrated Frontier Sciences, Department of Automotive Science, Kyushu University, Japan)

Theoretical and experimental study on the significance of electronegativity in a high entropy oxide photocatalyst

9:50

Edoardo Fabbrini (PhD student, Graduate School of Mathematics, Kyushu University, Japan)

Modeling, Analysis and Finite Element Simulations of Kinematically Incompatible von Kármán Plates

10:20

Sergei Manzhos (Associate Professor, Institute of Science Tokyo, Japan)

Large-scale electronic structure materials modeling with the help of machine learning-enhanced DFTB and OF-DFT

10:50

Yu Kaneko (Senior Research Scientist, Digital Strategy Center, Daicel Corporation, Osaka, Japan)

Cellulose Solvent Search by usage of Molecular Dynamics Simulation and Machine Learning

11:20-11:30 COFFEE BREAK

Session II: Materials Discovery for CO2 Capture: Experiments, Computational Chemistry, and AI
Chair: Linh T. H. Nguyen

11:30

Paul O'Brien (Associate Professor, York University, Canada)

Machine Learning for Direct Air Carbon Capture: Challenges and Opportunities

12:00

Tanay Sahu (PhD Student, York University, Canada)

A Comprehensive Life Cycle Assessment of Low- Temperature Direct Air Carbon Capture and Storage (LT-DACCS) Systems: Evaluating Global Warming Potential and Energy Requirements Across Diverse Regions

12:20

Victor Eke (Master's student, York University, Canada)

The Energy Challenge from a Materials Perspective

12:40

Yasser Salah Eddine Bouchareb (PhD Student, INRS, Université du Québec, Canada)

Optimization of Transition Metal Alloy Adsorbents for CO_2 Capture Using Machine Learning (ML) and Density Functional Theory (DFT).

13:00-14:00 LUNCH

Session III: Modeling and Calculations: From Atomic Structure to Applications
Chair: Jacqueline Hidalgo-Jiménez

14:00

Maryam Nurhuda (Postdoctoral Fellow, Institute for Integrated Cell-Materials Science (iCeMS), Kyoto University, Japan)

Can it be detected? A Computational Protocol for Evaluating Chemiresistive Sensor for Early Disease Detection

14:30

David Samuel Rivera Rocabado (Associate Graduate Professor, School of Advanced Science and Engineering, Hiroshima University, Japan)

Decoding and engineering catalytic activity: ESDA for CO adsorption and activation on Ru-based catalysts

15:00

Marcos Gomes Eleuterio da Luz (Professor,
Departamento de Física, Universidade Federal do Paraná – Curitiba, Brazil)

Basic Cells Special Features and Their Influence on Global Transport Properties of Long Periodic Structures

15:30

Karel Svadlenka (Professor,Tokyo Metropolitan
University, Japan)

Variational analysis of elastoplastic
deformation of structured materials

16:00

Tomonari Inamura (Professor,Institute of Science
Tokyo, Japan)

Designing long-life shape memory alloys using the triplet condition

Session IV: Quebec-Japan Collaboration, Closing Remarks, and Awards
Chair: Kulbir Ghuman

16:30

Emilie MIKURA (Emilie MIKURA (Attachée enrecherche,scienceetinnovation,Délégation
générale du Québec à Tokyo,Japan)

Quebec-Japan Collaboration

16:40

Adélie De Marre (Scientifique en résidence,
Soutenue par le Fonds de recherche du Québec, Délégation générale du Québec à Tokyo, Japan)

Quebec-Japan Collaboration

16:50

Oral Presentation Awards sponsored by Royal Society of Chemistry (RCS)

17:00

Organizers

Closing Remarks

17:15

LAB TOURS

申込方法

＼下記URLより参加登録をお願いいたします／

参加登録フォーム