3RD CEMDI-PAIMS SYMPOSIUM

ADVANCING MATERIALS DATA, DESIGN, & DISCOVERY

HOSTED BY

INTERNATIONAL INSTITUTE FOR CARBON-NEUTRAL ENERGY RESEARCH
&
INSTITUTE OF MATHEMATICS FOR INDUSTRY (IMI)

KYUSHU UNIVERSITY
JAPAN

DATE: APRIL 23-25, 2025
VENUE: I²CNER HALL C, ITO CAMPUS, KYUSHU UNIVERSITY

WEDNESDAY, APRIL 23RD, 2025
TIME: 9:30 AM – 5:20 PM (JST)

Time	Speaker	Affiliation	Title
Session I: Opening Remarks			**Chair: Aleksandar Staykov**
9:30 AM	Tatsumi Ishihara	Director, I²CNER, Kyushu University, Japan	Introduction to International Institute for Carbon-Neutral Energy Research (I2CNER)
9:40 AM	Kenji Kajiwara	Director, IMI, Kyushu University, Japan	Introduction to Institute of Mathematics for Industry (IMI)
9:50 AM	Quebec/Canada Delegate	Delegation of Quebec in Tokyo, Japan	Strengthening Quebec-Canada-Japan Ties for a Brighter Future in Sustainable Technologies

10:00 AM	Rusoma Akilimali	Technology and Innovation Advisor, PRIMA, QC, Canada	Promoting Québec-Japan Collaboration in Advanced Materials
10:10 AM	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
10:20 AM	Kulbir Ghuman Alex/Pierluigi	Director CEMDI and Associate Professor, INRS, Université du Québec, Canada PAIMS	Computational Energy Materials Design Infrastructure (CEMDI): Goals and Opportunities
10:30 – 10:40 AM COFFEE BREAK			
Session II: AI for Materials Discovery			**Chair: Pierluigi Cesana**
10:40 AM	Xiangdong Ding	Professor and Dean, School of Materials Science and Engineering, 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 AM	Tom Woo	Professor, University of Ottawa, ON, Canada	Machine Learning Assisted Design of Porous Materials for CO_2 capture using Integrated Atomistic Scale and Process Scale simulations
11:40 AM	Daniel Packwood	Associate Professor, Institute for Integrated Cell-Material Sciences (iCeMS), Kyoto University, Japan	Machine learning for functional molecular materials and supramolecular assemblies
Lunch 12:10 AM - 1:10 PM			
Time	**Speaker**	**Affiliation**	**Title**
Session III: AI for Materials Discovery			**Chair: Tsuneyuki Ozaki**
1:10 PM	Adroit Fajar	Assistant Professor, I2CNER,	Can AI Truly Revolutionize Molecular Design?

		Kyushu University, Japan	
1:40 PM	Adrian Xiao Bin Yong	Postdoctoral Fellow, I2CNER CESD, Kyushu University, Japan	Dismai-Bench: Benchmarking generative models using disordered materials
2:10 PM	El Tayeb Bentria	Researcher, Qatar Environment and Energy Research Institute, HBKU	Computational Materials Science in the Era of Large Language Models: Challenges and Opportunities
2:40 PM	Chandra Veer Singh	Professor, University of Toronto, Canada	AI-enabled discovery of high-entropy materials for electrochemical energy conversion and storage
3:10 -3:20 PM COFFEE BREAK			
Session IV: Computational Modelling for Electrochemical Devices			**Chair: David S. R. Rocabado**
3:20 PM	Jose C. M. Madrid	Postdoctoral Fellow, INRS, Université du Québec, Canada	Aluminium and Iron Impurity Segregation in Yttria-Stabilized Zirconia Grain Boundaries
3:50 PM	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
4:20 PM	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
4:50 PM	Tsuneyuki Ozaki	Professor, INRS-EMT, Canada	Intense terahertz field-induced impact ionization in narrow bandgap semiconductors
5:20 PM CLOSING			

THURSDAY, APRIL 24TH, 2025
TIME: 9:30 AM – 5:00 PM (JST)

Time	Speaker	Affiliation	Title
Session I: Computational Chemistry for Material Design			**Chair: Chandra V. Singh**
9:30 AM	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 AM	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 AM	Daniel Gueckelhorn	PhD student, INRS, Université du Québec, Canada	Density functional theory study of electrical properties of misfit dislocations in $SrTiO_3$
10:50 AM - 11:00 AM COFFEE BREAK			
Session II: AI for Materials Discovery			**Chair: Sergei Manzhos**
11:00 AM	Kazuki Yoshizoe	Professor, Research Institute for Information Technology, Kyushu University, Japan	Accelerating Molecular Discovery with Game AI methods and Supercomputers
11:30 AM	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 AM	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
Lunch 12:20 PM - 1:20 PM			

Session III: Modeling and Calculations: From Atomic Structure to Applications			**Chair: Linh T. H. Nguyen**
1:20 PM	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
1:50 PM	Ryuichi Tarumi	Professor, Osaka University, JP	Dislocation and disclination in crystalline materials: a differential geometry approach
2:20 PM	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
2:50 PM - 3:00 PM COFFEE BREAK			
Session IV: Accelerating Materials Discovery: New Approaches and methods			**Chair: Daniel Packwood**
3:00 PM	Linh Thi Hoai Nguyen	Assistant Professor, I2CNER, Kyushu University, Japan	Accelerating Material Discovery through an Automated and Data-Driven Workflow
3:30 PM	Natsuhiko Yoshinaga	Professor, Department of Complex and Intelligent Systems, Future University, Hakodate, Japan	Reinforcement learning for self-assembly problems
4:00 PM	Antoine Diez	Postdoctoral Fellow, Kyoto University, Japan	Multicellular simulations with shape and volume constraints using optimal transport
4:30 PM	Ettore Barbieri	Senior Researcher, JAMSTEC, Japan	Algorithms for Aggregation, Percolation, and Thermoelasticity in Pyroresistivity of Conductive Polymer Composites
CLOSING 5:00 PM / DINNER (6:00 PM – 8:00 PM)			

FRIDAY, APRIL 25TH, 2025

TIME: 9:30 AM – 5:30 PM (JST)

Time	Speaker	Affiliation	Title
Session I: Experimental Materials Science Supported by Computational Analysis			**Chair: Paul O'Brien**
9:30 AM	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 AM	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 AM	Fiorenzo Vetrone	Professor, INRS, Université du Québec, Canada	Frontiers in Rare Earth Doped Nanoparticles: Design, Properties, and Applications
10:50 AM	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 AM - 11:30 AM COFFEE BREAK			
Session II: Materials Discovery for CO_2 Capture: Experiments, Computational Chemistry, and AI			**Chair:**
11:30 AM	Paul O'Brien	Associate Professor, York University, Canada	Machine Learning for Direct Air Carbon Capture: Challenges and Opportunities
12:00 AM	Victor Eke	Master's 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 PM	Tanay Sahu	PhD Student, York University, Canada	Identification and evaluation of CO_2 photocapture materials

12:40 PM	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).
1:00 PM - 2:00 PM LUNCH *PM* *(Meeting with Directors- To be discuss)*			
Session III: Modeling and Calculations: From Atomic Structure to Applications Chair:			
2:00 PM	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
2:30 PM	David Samuel Rivera Rocabado	Associate Professor, Graduate School of Advanced Science and Engineering, Hiroshima University, Japan	Decoding and engineering catalytic activity: ESDA for CO adsorption and activation on Ru-based catalysts
3:00 PM	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
3:30 PM	Karel Svadlenka	Professor, Tokyo Metropolitan University, Japan	Variational analysis of elastoplastic deformation of structured materials
4:00 PM	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			
4:30 PM	Emilie MIKURA	Attachée en recherche, science et innovation,	Quebec-Japan Collaboration

		Délégation générale du Québec à Tokyo, Japan	
4:40 PM	Adélie De Marre	Scientifique en résidence, Soutenue par le Fonds de recherche du Québec, Délégation générale du Québec à Tokyo, Japan	Quebec-Japan Collaboration
4:50 PM	TBD	Trade Commissioner's office	TBC
5:00 PM	Organizers	To be decided	Closing Remarks
5:15 PM	Oral Presentation Awards sponsored by Royal Society of Chemistry (RCS)		
5:30 pm LAB TOURS			

WITH THE SUPPORT FROM THE FY2025 IMI JOINT USAGE INTERNATIONAL PROJECT RESEARCH-WORKSHOP (I): "PROMOTING MATERIALS DATA, DESIGN, AND DISCOVERY" (REFERENCE NO: 2025B007).