



Institut national
de la recherche
scientifique

The 2nd Annual CEMDI Symposium

27 - 29 May, 2024

Venue: Place Bonaventure
800 de La Gauchetière W.
Northwest Portal, Suite 6900
Montreal, Quebec H5A 1K6, Canada



CEMDI

Computational Energy
Materials Design
Infrastructure
www.cemdi.inrs.ca

Detailed Program

(K: Keynote, I: Invited, C: Contributed)

Day 1, 27th May, Monday

8:30 AM

Registration and Coffee

9:30 AM		Francois Legare	INRS-EMT, Université du Québec, Canada	Welcome Note
9:40 AM		Kulbir Ghuman	INRS-EMT, Université du Québec, Canada	CEMDI
9:50 AM		Chico Tongi	Toronto	A nod to art and science: Eco-conscious living

Session I: Advancements in Sustainable Materials and AI

Chair: Francois Vidal

10:00 AM	K	Normand Mousseau	Université de Montréal, Canada	Rethinking materials for a sustainable world
10:30 AM	I	Jonathan Shock	University of Cape Town, South Africa	Rich Embeddings and Deep Understanding "?"
11:00 AM	I	Laurent Karim Béliand	Queen's University, Canada	Machine-learning interatomic potentials through small-cell active learning: successes and challenges

11:30 AM

Coffee Break (10 min)

Session II: Data-Driven Innovations in Materials Science

Chair: Chandra Veer Singh

11:40 AM	I	Tom K. Woo	University of Ottawa, Canada	Flies in the ointment of materials databases: How common are structures with serious errors?
12:10 AM	I	Hartmut Schlenz	Forschungszentrum Juelich, Germany	Machine learning for the prediction of physical properties of cubic oxide perovskite
12:40 AM	I	Daniel Packwood	Kyoto University, Japan	Data science for stem cell science and bio-marker sensor research

1:10 PM

Lunch (1 hour)

Session III: Machine Learning for Catalyst Design

Chair: Alex Hernandez-Garcia

2:10 PM	I	Pierluigi Cesana	Kyushu University, Japan	Fully automatized optimization of ring-opening reactions in lactone derivatives via 2-step machine learning
2:40 PM	C	Parastoo Agharezaei	INRS-EMT, Université du Québec, Canada	CuNi-based single-atom alloy catalysts for nitrogen reduction reaction: A DFT study

3:00 PM	C	Mehdi Shamekhi	Concordia University, Canada	Machine learning assisted screening and DFT characterization of bimetallic alloy catalysts for the nitrogen reduction reaction
3:20 PM Coffee Break (20 min)				
Session IV: Computational Innovations in CO₂ Capture Technologies				Chair: Paul O'Brien
3:40 PM	I	Aleksandar Staykov	Kyushu University, Japan	Design of Direct Air Capturing Polymer Membranes Using First-principle Simulations and Machine Learning
4:10 PM	I	Josette El Haddad	National Research Council, Canada	Sensing solutions show the way for clean energy advances and decarbonised industries
4:40 PM	I	Conrard G. T. Feugmo	University of Waterloo, Canada	Computational screening for improved electrochemical CO ₂ capture
5:10 PM	C	Tanay Sahu	York University, Canada	Unlocking Metal Surface Charges for Green CO ₂ Capture: A First-Principle Study

Day 2, 28th May, Tuesday

Session I: Advancements in Sustainable Materials and AI				Chair: Sergei Manzhos
9:00 AM	I	Chandra Veer Singh	University of Toronto	Design and optimization of energy materials using high throughput DFT computations and AI techniques
9:30 AM	I	Linh Thi Hoai Nguyen	Kyushu University, Japan	Applied math for AI-driven design of photo-resisting polymers
10:00 AM	I	Hector Orozco, Bertha Vazquez, Julien Robitaille, Francis Quintal	Clemex Technologies Inc., Canada	Making automated image analysis simple with AI
10:30 AM	I	Alex Hernandez-Garcia	Mila, Université de Montréal, Canada	Crystal-GFN: generative machine learning to discover materials with desirable properties and constraints
11:00 AM Coffee Break (10 min)				
Session II: Data-Driven Innovations in Materials Science				Chair: Jonathan Shock
11:20 AM	I	Sergei Manzhos	Tokyo Institute of Technology, Japan	Hybrid approaches to machine learning from small datasets for applications from materials informatics to large-scale DFT
11:50 AM	I	Edern Menou	Safran Tech Inc., France	Machine-learning and thermodynamics-driven alloy design for high temperature aerospace applications
12:20 PM	I	Normand Mousseau	Université de Montréal, Canada	Challenges and advances in the modeling of activated processes: how focusing on energy surfaces allows to better understand the temporal evolution of physical systems

12:50	C	Zhiwen Chen	University of Toronto	Theoretical design of High entropy alloy catalysts
1:10 PM Lunch (1 hour)				
Session III: Machine Learning for Catalyst Design			Chair: Gabriel Antonius	
2:10 PM	I	Kirk H. Bevan	McGill University, Canada	The machine learning driven design of single atom alloys for catalysis through physically compressed electronic structure descriptors
2:40 PM	I	Takaya Fujisaki	Shimane University, Japan	A Strategy to Reduce the Activation Barrier in Methane Dissociation Reactions Using Ni Nanoparticles on CeO ₂ Based on First-Principles Calculation
3:10 PM	C	Xue Yao	University of Toronto, Canada	Structural Self-Regulation-Promoted NO Electroreduction on Single Atoms
3:30 PM	C	Samuel Lemay	UQTR (IRH), Canada	Simulations numériques de catalyseurs moléculaires pour la production d'hydrogène
3:50 PM Coffee Break (10 min)				
Session III: Computational Exploration of Thin Film Materials			Chair: Kirk Bevan	
4:00 PM	I	Grace Wei	Encellin Inc.	Polymeric thin film applications in healthcare: enabling living medicine.
4:30 PM	C	Brahim Ahammou	INRS-EMT, Université du Québec, Canada	Exploring SiN _x Thin Film Deposition and Mechanical Properties Through Molecular Dynamics
4:50 PM	C	Youssef Ouldhnini	INRS-EMT, Université du Québec, Canada	Composition-Structure-Mechanical Properties Relationship of Amorphous Hydrogenated Silicon Nitride
5:10 PM	C	Daniel Gueckelhorn	INRS-EMT, Université du Québec, Canada	Strain-induced enhancement of surface self-diffusion on strontium titanate (001) surfaces

Day 3, 29th May, Wednesday				
Session I: Advancements in Sustainable Materials and AI			Chair: Anderson Avila	
9:00 AM	I	Gabriel Antonius	Université du Québec à Trois-Rivières	Machine learning assisted canonical sampling for hydrogen storage materials
9:30 AM	C	Hao Sun	Queen's University, Canada	An interatomic potential for sodium and chlorine in both neutral and ionic states
9:50 AM	C	Nasim Soltani	INRS-EMT, Université du Québec, Canada	A Regularized Reputation Mechanism for Enhanced Fairness in Federated Learning

10:10 AM	C	Yasser Bouchareb	INRS-EMT, Université du Québec, Canada	Screening binary alloys for CO2 photo capture using GNN
10:30 AM	C	Jiapeng Zhang	University of Toronto	Dual Model Carbon Engineering in Kilogram-scale Si/C Composites for Stable Lithium Storage
10:50 AM	Coffee Break (10 min)			Chair: Tarek Djrefi
11:00 AM	I	Tayeb A. Denidni	INRS-EMT, Université du Québec, Canada	IEEE lecture
11:30 AM	I	Shervin Vakili	INRS-EMT, Université du Québec, Canada	IEEE Lecture
12:00 PM	RCS Oral Presentation Awards			
12:10 PM	Closing Remarks			