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

Institut national de la recherche scientifique

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 Béland	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 CO_2 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 CO2 capture
5:10 PM	C	Tanay Sahu	York University, Canada	Unlocking Metal Surface Charges for Green CO2 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 CeO2 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 SiNx 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,Universit é 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)**			
Session II: IEEE lectures				**Chair: Alain Pignolet**
11:00 AM	I	Clara Santato	Polytechnique Montreal, 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**			