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

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CEMDI
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Abstracts

Day 1, 27th May, Monday

Presenting Author:	Normand Mousseau
Affiliation:	Département de physique, Institut Courtois and Regroupement québécois sur les matériaux de pointe, Université de Montréal
Corresponding Author(s):	
Title:	Rethinking materials for a sustainable world

Abstract:
Our societies will have to build massively in the coming decades to meet the needs of a world population that is expected to increase by 25% by 2050, to reach 9.7 billion - and more than 11 billion in 2100. At the same time, our societies will have to adapt to climate change and profoundly transform our energy system to decarbonize it. Beyond reducing greenhouse gas emissions, it is essential that these infrastructures are as sustainable as possible in order to protect biodiversity and the environment. The responsibility for this objective lies not only in the hands of public decision-makers, architects and engineers, it must also concern materials science researchers. As I will try to demonstrate, this responsibility to rethink materials for a sustainable society must be seen as a positive challenge that gives way to fundamental science and applied science while creating a new dynamic between disciplines, and an integrated vision of the actions and choices we have to make every day.

Presenting Author:	Jonathan Shock
Affiliation:	University of Cape Town and INRS
Corresponding Author(s):	
Title:	Rich Embeddings and Deep Understanding (?)

Abstract:
The transformer architecture combined with multi-task learning gives the possibility of very rich embedding spaces. LLM's seem to build up amazing structures which encode relationships between concepts in ways that are ever-surprising. In this talk I will follow the logic of the Bitter Lesson and ask what we can do in the space of material science, beyond the realm of narrow tasks by seeing whether models can learn the deeper rules of physics at the atomic scale.

Presenting Author:	Laurent Karim Béland
Affiliation:	Queen's University
Corresponding Author(s):	LK Béland, Hao Sun, Aditya Kamath, Yu Luo, Yiwen Sun, Matt Thoms, Richard Meng, Jason Meziere, Gus Hart, Mark Daymond
Title:	Machine-learning interatomic potentials through small-cell active learning: successes and challenges

Abstract:
Training machine-learning interaction potentials (MLIP) has value in-as-much the computational cost of training the potential is smaller than the computational savings associated to using the MLIPs. Herein, we provide examples where a small-size cell approach, leveraging active-learning strategies, led to generating high-quality MLIPs based on DFT databases containing as few as a few hundred configurations, mostly comprised of one to eight atoms. In particular, we leverage the moment tensor potential (MTP) framework, albeit our findings should be generalizable to other MLIP formalisms. We will cover examples that include Zr, ZrFeNb compounds, Zr hydrides, Na-NaCl-Cl, Si-SiO2-O. We will present both the benefits and limitation of this approach.

Presenting Author:	Tom K. Woo
Affiliation:	University of Ottawa
Corresponding Author(s):	Tom K. Woo, Andrew White, Marco Gibaldi, Jake Burner, Alex Mayo
Title:	Flies in the Ointment of Materials Databases : How Common are Structures with Serious Errors ?

Abstract:
Metal organic frameworks (MOFs) are a class of crystalline nanoporous materials

constructed from both organic and inorganic building units. They have attracted attention in my fields of application but show particular promise in gas storage and separation applications where they have been commercialized. As with other materials, data-driven and machine learning materials discovery workflows are in widespread use in the MOF field. Databases of MOFs, some containing millions of structures, have proliferated recently. These databases of MOFs have been used for computational high-throughput screening and for developing machine learning models, where the training data is typically generated from compute intensive DFT calculations or other atomistic simulations performed on the structures. The implicit assumption in using these databases is that the structures therein are chemically reasonable. We have developed a novel method that computes the oxidation states of the metals to detect serious structural errors that are hard to identify using available automated tools. Using this tool we have screened over two million materials in various widely used MOF databases. Alarmingly, the most popular databases have structural error rates of almost 50%, and all but a select few databases have errors rates of 40% or more. The errors are such that the structures are not chemically sensible and therefore cannot be made in the lab. This puts into question the results of many computational screening and machine learning studies of MOFs that have utilized these databases. The implications of these findings will be discussed.

Presenting Author:	Hartmut Schlenz
Affiliation:	Forschungszentrum Juelich, IEK-1, Wilhelm-Johnen-Strasse, D-52425 Juelich, Germany
Corresponding Author(s):	Hartmut Schlenz
Title:	Machine learning for the prediction of physical properties of cubic oxide perovskite

Abstract:

The mineral perovskite, with the general composition ABX3, shows quite different physical properties due to the flexibility of its chemical composition and the occupation of positions A and B by different elements in the cubic crystal structure. These properties make perovskite particularly attractive for applications as an energy material in the field of renewable energies. For example, perovskite can be used as a magnetic material or as an electrical conductor and/or ion conductor, e.g. for the production of solar cells, for batteries, and for fuel cells. In this work we concentrated on oxide cubic perovskites ABO3 of different compositions, which are to be used as conductors in gas separation membranes for the production of pure hydrogen or oxygen, and additionally for applications in fuel cells. We used machine learning in order to demonstrate how even smaller training data sets are applicable for the precise and accurate prediction of suitable chemical compositions for the development of new ceramic gas separation membranes, avoiding any doping with toxic cobalt or expensive rare earths. For this purpose we have evaluated available experimental data, determined missing crystallographic information using bond-valance modeling and programmed a new Python code called PeCon.py, that generates the necessary training data sets. These data served as input for subsequent machine learning, and indeed, suitable compositions can be predicted this way. We also predicted the elastic properties for eighty different oxide perovskite phases. Since perovskites, e.g. for fuel cells, are often built up as multilayer ceramic systems, precise knowledge of the elastic properties of the various layers is of particular importance. Only in this way can the stability of such layer systems be predicted for higher temperatures, as greater stresses within the layers and also between the layers can lead to a disintegration of the materials. For this work we have collected and analyzed available experimental data and those from DFT simulations. Unfortunately, it has been shown that the available data do not allow the creation of a general model for the prediction of the elastic properties. Therefore, this time we went the opposite way, which means that we have used the available data all together as training data, filled gaps in the data records with the help of machine learning and finally used the results as an input for a newly written Python code called PeMod.py. This program is then able to accurately calculate the values for the cell constants, the elastic constants, the bulk modulus, the shear modulus, the Young's modulus, the Poisson’s ratio, the anisotropy and even the Vickers hardness for any desired composition within the given limits.

Presenting Author:	Daniel Packwood
Affiliation:	Kyoto University
Corresponding Author(s):	Daniel Packwood
Title:	Data science for stem cell science and bio-marker sensor research

Abstract:
Data science has rapidly diffused throughout chemistry and materials science over the last several years. This presentation will illustrate two applications of data science in these fields using examples from our group:

(i) Human breath contains over 1000 volatile organic compounds (VOCs), abnormal concentrations of which can indicate the presence of certain diseases. We examined whether any of these diseases could be detected using a new sensor architecture based on metal-organic framework metals (MOFs). To this end, we developed a new computational protocol to cheaply characterize the VOC-MOF interaction based upon density-of-states changes. Analysis of the resulting data using a statistical procedure then helped identify potential diseases which could be detectable.

(ii) The area of chemical biology is fraught with problems related to small data sizes. In a recent project, we succeeded to design a new bioactive compound (a WNT inhibitor for cardiac cell generation from stem cells) using a regression model trained on only 81 data points. To compensate for the small data set size, a new set of chemically rich molecular descriptors were developed, which incorporated both molecular conformation and hydrophilicity information. Model overfitting was avoided by studious use of sensitivity analyses. Application of the model to a virtual library of compounds led to the discovery of a new WNT inhibitor, whose ability was then confirmed in subsequent experiments.

Presenting Author:	Pierluigi Cesana
Affiliation:	Kyoto University
Corresponding Author(s):	
Title:	Fully automatized optimization of ring-opening reactions in lactone derivatives via 2-step machine learning

Abstract:
Cyclization and cycloreversion of organic compounds are fundamental kinetic processes in the design of functional molecules, molecular machines, and nano-switches. We present a fully automatic computational platform for the design of a class of 5- and 6-membered ring lactones by optimizing the ring-opening reaction rate. Starting from a minimal initial parent set, our program generates iteratively cascades of pools of candidate lactone derivatives where optimization and down-selection are performed not requiring human supervision at any stage. We use Density Functional Theory combined with transition state theory to elucidate the exact mechanism leading to the lactone ring opening. Based on the analysis of the reaction pathway and the frontier molecular orbitals, we identify a simple descriptor that can easily correlate with the reaction rate. The program is successful in identifying a large class of lactone derivatives with enhanced ring-opening properties. Our platform is modular and our current implementation for lactone could be further generalized to more complex systems via substitution of the quantum chemical and fingerprinting modules.

Presenting Author:	Parastoo Agharezaei
Affiliation:	INRS-EMT PhD student
Corresponding Author(s):	Prof. Kulbir Ghuman
Title:	CuNi-based single-atom alloy catalysts for nitrogen reduction reaction: A DFT study

Abstract:
Searching for efficient, active, and stable catalysts for the nitrogen reduction reaction (NRR) is vital to substitute the traditional Haber–Bosch process which accounts for 1-2% of global energy consumption and emits 300 millions of CO2 per year. The other sustainability problems of Haber–Bosch process are the required energy for H2 production, and handling the unreacted gas recycles. The catalytic NRR is one of the most

promising reactions to produce ammonia (NH3) under milder conditions with lower energy use and less greenhouse gas emission. However, the lack of effective catalysts remains the major obstacle for the practical applications of NRR. Alloys have been demonstrated as potential ammonia production catalysts in the literature. However, for alloys to be commercially viable, one needs to improve their catalytic activity for N2 reduction by strategically manipulating the several unique active sites present on their surface. Herein, by using computational tools, we initially created the Cu0.5Ni0.5 alloy via Special Quasi Random Structure (SQS) and Genetic Algorithm (GA) which showed 21 times higher catalytic activity than Cu and 3 times higher activity than Ni catalysts for NRR. Position and concentration of Ni atoms around different active sites and orientation of N2 molecule (end-on or side-on adsorption modes) play an important role in determining the activity of the catalyst. In order to further improve the catalytic activity of the CuNi catalysts recently we systematically investigated transition metal-doped CuNi-based single-atom alloys (SAA). More specifically, we evaluated CuNi catalysts doped with Au, Ag, Pd, Pt, Co, Ru and Fe. Our study showed that Au, Ag and Pd doped CuNi(111) SAA exhibited a reduced energy barrier of ~0.4 eV in the first hydrogenation step (the rate limiting step) as compared to that of the CuNi(111). This work provides pathway to design high performance catalysts for NRR.

Presenting Author:	Mehdi Shamekhi
Affiliation:	Department of Physics, Concordia University
Corresponding Author(s):	Arash Toghraei , Daniel Guay, and Gilles H. Peslherbe
Title:	Machine learning assisted screening and DFT characterization of bimetallic alloy catalysts for the nitrogen reduction reaction

Abstract:

The production of ammonia via the environmentally friendly electrochemical nitrogen reduction reaction (NRR) faces two major challenges, low catalytic activity and low selectivity. The low activity is the result of poor nitrogen adsorption on the surface of the catalyst (a non-electrochemical step) while the selectivity issue is due to the competing hydrogen evolution reaction (which diverts most of the current from ammonia production). The d-band model offers simple, yet effective, means to evaluate the activity and selectivity of transition metal surfaces, and judicious alloying allows to tune the d-band of transition metals favorably. However, determining the optimal composition and structure of alloys for catalysis remains experimentally and even computationally challenging and demanding. In this work, we use machine learning algorithms for preliminary screening of bimetallic alloy surfaces with different stoichiometric ratios. The d-band features of various metal surfaces calculated by density-functional theory (DFT) along with intrinsic characteristics of the adsorption sites were used as surface descriptors to train the machine learning algorithms. The promising alloys were further investigated through DFT

characterization of the reaction free energy profiles in order to determine the potential limiting step of the NRR and assess the feasibility of the reaction by estimating the theoretical overpotential.

Presenting Author:	Aleksandar Staykov
Affiliation:	International Institute for Carbon Neutral Energy Research (WPI-I2CNER), Kyushu University, JApan
Corresponding Author(s):	
Title:	Design of Direct Air Capturing Polymer Membranes Using First-principle Simulations and Machine Learning

Abstract:

We employ density functional theory to investigate the binding interaction between polydimethylsiloxane and CO2 for application in gas separation membranes. The binding strength has been studied systematically as a function of the monomer conformational rotations in the polymer chain. Our work identified major differences between the CO2 interaction with the helical conformation and the linear conformation of polydimethylsiloxane polymer chains. We have further estimated dependence between the CO2 binding strength and the polydimethylsiloxane polymer chain curvature by systematically evaluating the CO2 binding to cyclic polydimethylsiloxane oligomers. The enhanced CO2 interaction with helical chains and cyclic oligomers was attributed to cooperative, confinement effects, and local electron density distribution at the Si–O–Si fragments. The binding modes were identified using vibration frequency analysis. We perform systematic computational mutation of polydimethylsiloxane to identify the physical descriptors which govern its CO2 selective interaction. Finally, an automatized algorithm was designed for computational crosslinking of polydimethylsiloxane which combined with machine learning is expected to lead to direct air capturing membranes with enhanced CO2 selectivity and permeability.

Presenting Author:	Josette El Haddad
Affiliation:	National Research Council Canada
Corresponding Author(s):	Josette El Haddad, Paul Bouchard, Christian Padioleau, Francis Vanier, Elton Soares de Lima Filho, Mohamad Sabsabi, Aïssa Harhira
Title:	Sensing solutions show the way for clean energy advances and decarbonised

	industries

Abstract:
The Clean Energy Innovation (CEI) Research Centre at the National Research Council Canada (NRC) is working on accelerating Canada's transition towards a thriving net-zero economy by the development of cutting-edge technologies. These new, game-changing approaches form a technological space that enables pioneering solutions for net-zero energy, critical minerals, advanced materials and industrial decarbonization. In this regard, the Optical Technology team of the CEI Research Centre, under the support of the Clean Production Program, is devising leading-edge optical sensors for real-time and on-site process monitoring to advance industry decarbonization, carbon management and critical minerals value chains.

In this talk, we will present an overview of industrial sensing applications that integrates standoff sensing with machine learning, that support activities related to carbon mineralization and critical minerals characterization and processing. A focus will be made on a unique Laser-Induced Breakdown Spectroscopy (LIBS) solution tailored to meet geologists' needs for on-site carbon sequestration assessment in geological matrices. The latest findings on carbon quantification and on the identification of factors involved in the sequestration of carbon in geological matrices, such as soil, tailings and rocks, will be discussed.

Presenting Author:	Conrard Giresse Tetsassi Feugmo
Affiliation:	University of Waterloo
Corresponding Author(s):	
Title:	Computational screening for improved electrochemical CO2 capture

Abstract:
The quest for net-zero emissions has catalyzed the evolution of carbon capture, storage, and utilization (CCUS) initiatives. Traditional CO2 capture techniques, notably those employing amine-based solutions to treat power plant emissions, are being reassessed due to their significant energy demands and inefficiencies related to Carnot limits during thermal regeneration. In pursuit of more sustainable alternatives, this study delves into the burgeoning field of electrochemical carbon capture concentration (eCCC) systems. These novel systems, which function at ambient conditions and are amenable to renewable energy sources, can potentially diminish the carbon capture processes' energy footprint. Central to our research is the computational design and analysis of sp2 amines for electrochemical CO2 sequestration, harnessing pH swing techniques. We investigate sp2 amine molecules, characterized by their redox activity, for their utility in eCCC, assessing their solubility, redox potential compatibility with aqueous environments, and the reversibility of their electrochemical reactions. The integration of AI in computational molecule screening further refines the selection process, pinpointing candidates most likely to enhance the efficiency and scalability of eCCC technology.

Presenting Author:	Tanay Sahu
Affiliation:	York University
Corresponding Author(s):	
Title:	Unlocking Metal Surface Charges for Green CO2 Capture: A First-Principle Study

Abstract:

The Net Zero by 2050 report by the IEA purports that CO2 capture from industrial processes and directly from air will play a critical role in achieving net-zero emissions. Liquid amine solutions are predominantly used for CO2 capture. However, regenerating these solutions requires energy-intensive, temperature, and pressure alterations, which lowers the efficiency and increases the costs of CO2 capture. Recently, research efforts have focused on developing solid adsorbents for CO2 capture. The energy penalty for regenerating solid adsorbents is low due to their low heat capacity. Herein, research is directed towards developing solid adsorbents that use a photo-desorption mechanism to capture CO2 with exceptionally high efficiency. These materials readily adsorb CO2 in the dark or under low-illumination conditions and photo-desorb CO2 when subjected to incident light. By using light as a “photoswitch” to desorb CO2, the need for energy-intensive pressure or temperature alterations is mitigated. This study employs density-functional theory calculations to examine the interaction between CO2 molecules and a diverse set of metal surfaces under varying charge conditions, encompassing both plasmonic and non-plasmonic transition metals, including Cu, Zn, Co, Fe, V, Pt, Ni, and Al. Our objective is to comprehensively understand how surface charges impact CO2 adsorption and desorption processes. Key factors under investigation include CO2 adsorption energy, the d-band center of pristine metal surfaces, surface charge distributions, and structural changes in CO2 upon adsorption. Materials that exhibit a high binding energy in the dark and a low binding energy in the light are promising candidates for photo-driven adsorbents for CO2 capture. Our findings emphasize that the d-band center of metal surfaces is an insufficient descriptor for CO2 adsorption and desorption. Different metals exhibit distinct behaviors in response to surface conditions when it comes to CO2 adsorption and desorption. Specifically, this study concludes that the metals that display optimum CO2 adsorption and desorption efficiency include Cu, Zn, Co(alpha), and Al(beta). CO2 adsorption on these metal surfaces occurs under neutral conditions, while desorption occurs in electron-rich or electron-deficient conditions. These findings have implications for future experimental studies aiming to manipulate CO2 interactions with neutral or charged metal surfaces, potentially driving innovative advancements in CO2 capture technologies.

Day 2, 28th May, Tuesday

Presenting Author:	Chandra Veer Singh
Affiliation:	Department of Mechanical and Industrial Engineering University of Toronto
Corresponding Author(s):	
Title:	Design and optimization of energy materials using high throughput DFT computations and AI techniques.

Abstract:

New materials are required to improve the efficiency and cost of renewable energy conversion technologies. However, the development of new materials often takes many years. In this regard, artificial intelligence (AI) techniques have emerged as new paradigm for materials development as they can reduce this materials discovery-deployment cycle by finding hidden patterns in material behavior and allow quick computational screening of promising material designs to guide experimentation.

In this talk, we would describe the role of data sciences, particularly machine learning, coupled with atomistic simulations, to design and explore novel materials for sustainable energy applications. The following representative examples will be discussed: (a) atomic catalysts to enable efficient CO2 reduction; (b) new electrolytes for all solid-state batteries; and (c) AI enabled design of high entropy alloy (HEA) catalysts for key energy conversion technologies key: CO2 reduction to useful chemical fuels, green ammonia production, and hydrogen evolution reaction. We will also discuss concurrent challenges and prospects of data science in energy materials development. These works will also serve as an example of how we can combine data science with atomistic modeling and experimental testing to design next-generation materials to combat global warming.

Presenting Author:	Linh Thi Hoai Nguyen
Affiliation:	International Institute for Carbon-neutral Energy Research, Kyushu University
Corresponding Author(s):	Pierluigi Cesana, Aleksandar Staykov
Title:	Applied math for AI-driven design of photo-resisting polymers

Abstract:

We present a fully automatized computational platform for the design of photo-resisting polymers by optimizing the ring-opening reaction rate. This is a general platform that aims at accelerating material discovery process by incorporating data-driven approach and quantum chemistry calculation in an automatic loop that required no-human interference during the iteration process. Starting from a minimal initial parent set, our graph-based evolutionary generative algorithm generates a large pool of candidates. We then use

Density Functional Theory (DFT) combined with transition state theory to elucidate the exact mechanism of ring opening reaction. A surrogate model is constructed based on the experimental data to estimate the ring opening reaction rate through some measurements that are easily obtained from DFT calculations. The measured data resulting from DFT calculations are used to construct Graph convolutional Neutral Network (GcNN) models to predict the ring opening reaction rate. Based on the prediction of the models, the optimization module down selects a list of potential good structures as the parents for the next iteration step. At the end of the automatized platform, we derive a list of candidates for further synthesize in the laboratory.

Presenting Author:	Hao Sun
Affiliation:	Queen's University
Corresponding Author(s):	Laurent Karim Béland
Title:	An Interatomic Potential for Sodium and Chlorine in both Neutral and Ionic States

Abstract:

Using a small-cell active learning approach, we generate a moment tensor potential (MTP) trained on only 609 configurations, jointly describing solid/liquid Na, gase-ous Cl, and crystalline/molten NaCl. This MTP implicitly captures the effect of atomic charge variations on energies and forces based on local atomic configura-tions. Extensive testing of this potential points to a high-fidelity description of the structural and transport properties of Na and NaCl. Furthermore, this potential was used to calculate the standard reduction potential and solubility limit of Na in mol-ten NaCl. These computed properties are in good agreement with available experi-mental data and ab initio calculations. Our proposed approach can be utilized to pre-dict the electrochemical and physical properties of molten salts with arbitrary com-positions and solutes.

Presenting Author:	Hector Orozco
Affiliation:	Clemex Technologies
Corresponding Author(s):	Hector Orozco, Bertha Vazquez, Julien Robitaille, Francis Quintal
Title:	Making automated image analysis simple with AI

Abstract:

Advances in computer vision and machine learning have not uniformly permeated the realm of materials microscopy, especially optical microscopy.

While certain fields employ sophisticated AI techniques that aim to be reproducible, robust, and validated, many metallography laboratories still suffer with methodologies that are time-consuming, lack reproducibility and robustness, and demand a high level of expertise in computer vision and/or AI from materials specialists.

For instance, methods such as point counting and manual intercept determination are laborious and often yield inaccurate or unreproducible results. A case is made with dendrite arm spacing measurements in aluminum castings.

Despite the industry's widespread adoption of threshold-based methods for automated image analysis, these techniques frequently falter due to their reliance on skilled computer vision professionals for development and their susceptibility to issues of reproducibility and accuracy from variations in illumination, sample preparation, and microstructure.

To address this issue, we propose two complementary approaches. Firstly, the creation of foundational models for image analysis that are robust to common variations in microscopy, sample preparation and generalize to most microstructure variations observed within a given domain. An example of this approach is grain size measurement in optical microscopy, where a foundational model is being developed and is presented herein.

Secondly, we emphasize the importance of addressing niche cases where the unique characteristics of the problem does not justify the large investment required for creating foundational models. In this case, we posit that the democratization of machine learning development through user-friendly, no-code tools with minimal learning curves is pivotal to fostering the adoption of automation in metallography laboratories. An example is provided by Clemex Studio, which shows the potential of this approach.

Presenting Author:	Alex Hernandez-Garcia
Affiliation:	Mila, Université de Montréal
Corresponding Author(s):	Alex Hernandez-Garcia
Title:	Crystal-GFN: generative machine learning to discover materials with desirable properties and constraints

Abstract:
The discovery of novel solid-state materials, such as electrocatalysts, super-ionic conductors, or photovoltaic materials, plays a critical role in addressing various global challenges. It has, for instance, the potential to significantly improve the efficiency of renewable energy production and storage, thereby making substantial contributions to climate crisis mitigation strategies. In this paper, we introduce Crystal-GFN, a generative model of crystal structures possessing desirable properties and constraints. Operating as a multi-environment, continuous-discrete GFlowNet, it sequentially samples structural attributes of crystalline materials, namely space group, composition and lattice

parameters. This domain-inspired approach enables the flexible incorporation of physicochemical and geometric hard constraints. We demonstrate the capabilities of Crystal-GFN to efficiently discover diverse and valid crystals with various properties: low predicted formation energy (median -3.2 eV/atom), band gap close to a target value and high density. Overall, Crystal-GFN is a crystal generation method that addresses several existing challenges in the literature and opens promising paths for accelerating materials discovery with machine learning.

Presenting Author:	Sergei Manzhos
Affiliation:	Tokyo Institute of Technology
Corresponding Author(s):	Manabu Ihara
Title:	Hybrid approaches to machine learning from small datasets for applications from materials informatics to large-scale DFT

Abstract:
Machine learning methods have firmly established themselves in the field of computational materials science. They are used and for the prediction of materials properties (materials informatics) and to improve (the speed or accuracy of) modeling methods. While some proposed computational workflows are rather complex, at the core of many of them, specifically for regression-type problems, lie feed-forward neural networks (NN) and kernel regression based methods. These methods have their advantages and disadvantages, such as the large number of nonlinear parameters in neural networks or difficulties with using large training sets with kernel methods. In many applications, descriptor spaces are high-dimensional, aggravating these problems as well as posing the problem of low data density even when the number of data is large. I will present our recent developments of hybrid methods combining the advantages and palliating the disadvantages of both types of methods (i.e. NNs and kernel methods). Examples from materials informatics and kinetic energy functional construction will be given.

Presenting Author:	Edern Menou
Affiliation:	Safran
Corresponding Author(s):	
Title:	Machine-Learning and Thermodynamics-driven Alloy Design for High Temperature Aerospace Applications

Abstract:
For decades, alloy design has been central to yielding technological improvements in

structural applications in the aerospace industry. New high performance alloys are much needed as material requirements, regulations and socio-economic expectations tighten. This talk will focus on work conducted at Safran Tech, Safran's corporate research center, on the development on new nickel-, titanium- and aluminium-based alloys for applications in gas turbines and around. Such complex applications embody many aspects of the usual compromises in material design: alloys are subject to wide temperature ranges, a variety of severe mechanical loads, and aggressive environments, the combination of these factors leading to an increasingly complex service life.

While regulations tighten, improvements made during the last few decades in numerical modelling and hardware allow for much broader design considerations. In the field of material sciences, concepts advocated through the Material Genome Initiative or Integrated Computational Material Engineering are meant to make use of such advancements, by proposing the integration of as much multi-scale, multi-physics modelling as possible to accelerate the introduction in service of novel materials. Hardware improvements also lead to the popularisation of Machine Learning, and more recently Deep Learning methods, which are useful to complement classical modelling approaches.

This talk will introduce the problem of alloy design as well as that of accelerated alloy development and experimental validation from the perspective of an engine manufacturer, and show through several use cases how a relatively simple, integrated ML-aided methodology can lead to innovative materials with original combinations of properties in a relatively short span of time. The many limitations of such system, the foremost issue being data availability, will also be discussed, as will prospective methodological enhancements and applications of Deep Learning in alloy design.

Presenting Author:	Normand Mousseau
Affiliation:	Département de physique, Institut Courtois and Regroupement québécois sur les matériaux de pointe, Université de Montréal
Corresponding Author(s):	
Title:	Challenges and advances in the modeling of activated processes: how focusing on energy surfaces allows to better understand the temporal evolution of physical systems

Abstract:

We employ density functional theory to investigate the binding interaction between polydimethylsiloxane and CO2 for application in gas separation membranes. The binding strength has been studied systematically as a function of the monomer conformational rotations in the polymer chain. Our work identified major differences between the CO2

interaction with the helical conformation and the linear conformation of polydimethylsiloxane polymer chains. We have further estimated dependence between the CO2 binding strength and the polydimethylsiloxane polymer chain curvature by systematically evaluating the CO2 binding to cyclic polydimethylsiloxane oligomers. The enhanced CO2 interaction with helical chains and cyclic oligomers was attributed to cooperative, confinement effects, and local electron density distribution at the Si–O–Si fragments. The binding modes were identified using vibration frequency analysis. We perform systematic computational mutation of polydimethylsiloxane to identify the physical descriptors which govern its CO2 selective interaction. Finally, an automatized algorithm was designed for computational crosslinking of polydimethylsiloxane which combined with machine learning is expected to lead to direct air capturing membranes with enhanced CO2 selectivity and permeability.

Presenting Author:	Zhiwen Chen
Affiliation:	University of Toronto
Corresponding Author(s):	Chandra Veer Singh
Title:	Theoretical design of High entropy alloy catalysts

Abstract:
Although research on high entropy alloy (HEA) catalysts is just coming to the forefront, the reported catalytic performance of HEA catalysts is better than almost all metal and alloy systems. This phenomenon raises two noteworthy issues: (i) Why do HEA catalysts have such excellent catalytic performance? (ii) How can the catalytic performance be further improved? To address these two issues, we studied the structure–property–performance relationships oof HEA catalysts, which is the biggest challenge for HEA catalysts with complex active sites and vast chemical space. Therefore, the research strategy for HEA catalysts should be shifted from exploring HEA catalysts through ‘trial and error’ or ‘directed research’ approaches to rationally designing HEA catalysts with optimal catalytic performance for a particular reaction.

Presenting Author:	Kirk H. Bevan
Affiliation:	McGill University
Corresponding Author(s):	Javad Shirani, Julio J. Valdés, Alain B. Tchagang, and Kirk H. Bevan
Title:	The machine learning driven design of single atom alloys for catalysis through physically compressed electronic structure descriptors

Abstract:

Javad Shirani 1, Julio J. Valdés 2, Alain B. Tchagang 2, and *Kirk H. Bevan 1,2
1 Division of Materials Engineering, Faculty of Engineering, McGill University, Canada
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Keywords: Single atom alloys, Surface Catalysis, Electronic Structure, Machine Learning

In this talk we discuss how the design of single atom alloys might be guided through electronic structure descriptors via machine learning methods. In particular, through the Sabatier principle we examine the contrasting efficacy of surface and adsorbate based electronic structure properties in predicting the catalytic activity of CO interaction within a wide range of single atom alloys. Two key findings result from this exploration. First, the adsorbate binding properties of single atom alloys are shown to be remarkably transferable even between alloyed substrates that are chemically distinct. Second, in terms of machine learning driven design prediction, the use of adsorbate based electronic structure descriptors is shown to markedly exceed conventional substrate-based descriptors (i.e., following from News-Anderson models of catalysis). Moreover, physically extracted adsorbate-based electronic structure properties are shown to maintain high predictive capacity even when approaching the intrinsic dimensionality of the catalysis subspace, to such a degree that they can even exceed machine learning generated feature compression methods. These findings not only highlight the importance of machine learning in guiding the prediction of alloys in catalysis applications, but that through the judicious use of physical insights the machine learning feature space can be compressed to arrive at more intuitive prediction approaches. In general, this work serves to further bridge conventional electronic structure methodologies in catalysis with emerging machine learning driven alloy design methods [1,2].

References:

1) J. Shirani, H. D. M. Pham, S. Yuan, A. B. Tchagang, J. J. Valdés, and K. H. Bevan, J. Phys. Chem. C 127, 12055 (2023).
2) J. Shirani, A. B. Tchagang, J. J. Valdés, and K. H. Bevan, J. Phys. Chem. C 128, 4483 (2024).

Presenting Author:	Takaya Fujisaki
Affiliation:	Shimane University
Corresponding Author(s):	
Title:	A Strategy to Reduce the Activation Barrier in Methane Dissociation Reactions Using Ni Nanoparticles on CeO2 Based on First-Principles Calculation

Abstract:
Biomass, a type of renewable energy, can be converted into methane, i.e., a hydrogen carrier, by anaerobic fermentation. The catalyst that has shown promise in recent years for improving the efficiency of the dry reforming of methane (DRM) reaction is CeO2 supported with Ni nanoparticles, and this study focused on the methane dissociation reaction (CH4→CH3-+H+), which is considered to have a particularly large activation energy in the reaction process of the DRM reaction. To understand the reaction mechanism and discuss how to reduce the activation energy, the methane dissociation at multiple Ni sites was evaluated by density functional theory (DFT). In addition, an experimental DRM reaction was performed using a Ni supported CeO2 flower-like catalyst to determine the activation energy for methane dissociation based on the rate of methane consumption. The results showed that the experimental value was 0.69 eV (15.91 kcal/mol), while the DFT value was 0.80 eV (14.45 kcal/mol), both very close to each other, providing validity to our calculation. Also, the DFT results indicate that Ni nanoparticles should be charged more positively so as to lower the activation energy for methane dissociation. The results of the study above provide a better understanding of the reaction mechanism and factors controlling the activation energy in the methane dissociation reaction, and provide insight into effective catalyst design for the DRM reaction.

Presenting Author:	Xue Yao
Affiliation:	University of Toronto
Corresponding Author(s):	
Title:	Structural Self-Regulation-Promoted NO Electroreduction on Single Atoms

Abstract:
Simultaneously elevating loading and activity of single atoms (SAs) is desirable for SA-containing catalysts, including single-atom catalysts (SACs). However, the fast self-nucleation of SAs limits the loading, and the activity is confined by the adsorption-energy scaling relationships on monotonous SAs. Here, we theoretically design a novel type of SA-containing catalyst generated by two-step structural self-regulation. In the thermodynamic self-regulation step, divacancies in graphene spontaneously pull up SAs from transition metal supports (dv-g/TM; TM = fcc Co, hcp Co, Ni, Cu), leading to the expectably high loading of SAs. The subsequent kinetic selfregulation step involving an adsorbate-assisted and reversible vacancy migration dynamically alters coordination environments of SAs, helping circumvent the scaling relationships, and consequently, the as-designed dv-g/Ni can catalyze NO-to-NH3 conversion at a low limiting potential of −0.25 V vs RHE.

Presenting Author:	Samuel Lemay

Affiliation:	UQTR (IRH)
Corresponding Author(s):	Gabriel Antonius
Title:	Simulations numériques de catalyseurs moléculaires pour la production d’hydrogène

Abstract:
Les catalyseurs moléculaires peuvent être utilisés afin d’améliorer de façon significative l’efficacité de la réaction d’évolution d’hydrogène (HER) dans les systèmes d’électrocatalyse et de photocatalyse [1,2]. Nous étudions une classe de catalyseurs sans métaux nobles composés d’un métal de transition et de deux ligands organiques de formule chimique M(L) 2 où M=Co, Cu, Ni. Cette classe de molécules possède de bonnes propriétés catalytiques à la fois pour l’électrocatalyse et la photocatalyse [3,4]. Nous utilisons la théorie de la fonctionnelle de la densité, afin de simuler pour plusieurs de ces catalyseurs les différents cycles catalytiques possibles. Ces calculs nous permettent ainsi de déterminer quels sont les cycles énergétiquement favorables et quelles sont les étapes limitantes. Nous utilisons le logiciel Orca afin de déterminer l’énergie électronique, les contributions des différents modes de vibrations à l’énergie libre et l’effet du solvant.

[1] S. Anwar, F. Khan, Y. Zhang and A. Djire, International Journal of Hydrogen Energy, 2021.
[2] J. Corredor, M. J. Rivero, C. M. Rangel, F. Gloaguen and I. Ortiz, Journal of Chemical Technology & Biotechnology, 2019, 94, 3049–3063.
[3] S.-P. Luo, L.-Z. Tang and S.-Z. Zhan, Inorganic Chemistry Communications, 2017, 86, 276–280.
[4] S. Rajak, O. Schott, P. Kaur, T. Maris, G. S. Hanan and A. Duong, Polyhedron, 2020, 180, 114412.

Presenting Author:	Grace Wei
Affiliation:	Encellin
Corresponding Author(s):	
Title:	Polymeric thin film applications in healthcare: enabling living medicine.

Abstract:
Half of the world's population lives with chronic disease. Treatment often means managing a regimen of medications. Beyond the problem of patient adherence to a drug regimen, drug kinetics usually do not respond dynamically to the body's condition. Cell therapy offers the promise of functional cures that restore activity in ways not achievable with drugs alone. Imagine the equivalent of transplants, but on an expanded menu. The safe delivery of cell therapy, however, is an obstacle that is still under study. Encellin's

clinical trial in Montreal with encapsulated cells is a first, using a thin film device that overcomes the key failure point in this field, the reaction to implanting foreign bodies, while supporting diffusion requirements for successful engraftment.

Presenting Author:	Brahim Ahammou
Affiliation:	INRS
Corresponding Author(s):	Brahim Ahammou, Youssef Ouldhnini, Kulbir Ghuman, Mohamed Chaker
Title:	Exploring SiNx Thin Film Deposition and Mechanical Properties Through Molecular Dynamics

Abstract:

Our study offers a comprehensive analysis of the mechanical properties of silicon nitride (SiNx) thin films. Utilizing molecular dynamics simulations, we explored atomic-level interactions and the structural evolution of SiNx thin films across various stoichiometries, temperatures, and deposition energies, mirroring the conditions of diverse deposition processes. This method enables accurate simulation of the deposition environment for low-hydrogenated SiNx films. To enhance computational efficiency, our simulations omit hydrogen due to its evaporation in chemical vapor deposition processes and its negligible impact on the dynamics of ion bombardment. We focused on the interactions between Si and N, which are crucial for determining the structural and mechanical properties of SiNx films. By employing three-body potentials, our simulations provide insights into the angular dependencies and interactions between atoms, thus shedding light on the film's microstructural development without the direct simulation of chemical reactions. Our methodology aims to clarify how microstructural features, such as bond distributions and density variations, influence the films' macroscopic mechanical properties, including intrinsic stress, Young's modulus, and fracture toughness. These insights are vital for understanding the mechanical stability of SiNx films in photonic applications. Linking simulation results with experimental characterizations, achievable through X-ray diffraction techniques, nanoindentation, and wafer curvature is possible. This research not only enhances our comprehension of the growth of SiNx films but also presents a framework for optimizing deposition processes to improve film durability against mechanical failures. Combining simulation with experimental characterizations, we have a comprehensive strategy for developing SiNx films with specialized properties for photonic applications.

Presenting Author:	Youssef Ouldhnini
Affiliation:	Institut National de la Recherche Scientifique (INRS)

Corresponding Author(s):	Youssef Ouldhnini
Title:	Composition-Structure-Mechanical Properties Relationship of Amorphous Hydrogenated Silicon Nitride

Abstract:
The mechanical properties of hydrogenated amorphous silicon nitride (a-SiN:H) thin films undergo significant alterations due to the incorporation of hydrogen. To gain deeper insights into this behavior, we employed molecular dynamics (MD) simulations to explore a-SiN:H systems with varying hydrogen concentrations. By processing the samples using the melt-quench method, our investigation primarily focused on elucidating the structural properties, including short- and medium-range atomic configurations, and correlating them with the mechanical responses of a-SiN:H systems containing diverse hydrogen amounts. Notably, through comprehensive analyses of pair distributions, angle distributions, coordination analysis, elastic constants, and stress-strain responses, we demonstrate that a low hydrogen fraction incorporated into silicon nitride reduces the number of undercoordinated atoms and consequently the concentration of dangling bonds. Conversely, high fractions of hydrogen lead to the depolymerization of the film network. These structural changes directly impact the material's strength by reducing the rigidity of a-SiN:H with increasing hydrogen content.

This work elucidates the intricate structure-mechanical properties relationships in a-SiN:H through atomistic simulations, providing valuable insights for understanding crack initiation and mechanical failures during experimental thin film deposition processes, especially for the low-pressure chemical vapor deposition technique employed in industrial applications.

Presenting Author:	Daniel Gueckelhorn
Affiliation:	INRS-EMT
Corresponding Author(s):	Daniel Gueckelhorn, Alfred Kersch, Andreas Ruediger
Title:	Strain-induced enhancement of surface self-diffusion on strontium titanate (001) surfaces

Abstract:
We present a numerical investigation of self-diffusion on strontium titanate TiO2-terminated (001) surfaces via density functional theory. The motivation for these simulations is based on the possibility of producing 1µm wide atomically flat strontium titanate TiO2-terminated terrace steps. To achieve such large steps strontium titanate was deposited on magnesium oxide with a resulting lattice mismatch of 7.9 %. A detailed model to explain the impact of strain on the self surface-diffusion is still missing. That is why we present the first detailed surface self-diffusion model for TiO2-terminated strontium titanate surfaces including effects occurring under equi-biaxial strain. Our

calculations indicate that Ti has the highest diffusion barrier with approximately 2.20 eV, thus representing the rate-limiting step for surface self-diffusion. Furthermore, the higher energy barriers of O and Ti in comparison to O2 and TiO2 indicate electronic activity with the surface atoms. Under the consideration of equi-biaxial strain as it would be encountered in e.g. heteroepitaxial thin films, the diffusion barriers for surface self-diffusion decrease for both compressive and tensile strains between –6 % and 2 %. For larger strains, we observe plastic deformations. This possibility to lower the energy barrier paves the way for accelerated and possible new mechanisms of surface diffusion and reconstruction of strontium titanate structures in a wide range of applications.

Day 3, 29th May, Wednesday

Presenting Author:	Gabriel Antonius
Affiliation:	Université du Québec à Trois-Rivières
Corresponding Author(s):	Gabriel Antonius
Title:	Machine learning assisted canonical sampling for hydrogen storage materials

Abstract:
Several key properties of materials for energy applications depend critically on temperature, and their prediction from numerical simulations requires a canonical sampling of the atomic configurations. Density functional theory (DFT) provides the most precise description of materials at the atomic scale, and it can be employed in ab initio molecular dynamics (AIMD) to attain a finite-temperature sampling of the configurations. However, its numerical cost limits the system size and the time over which a material can be simulated. On the other hand, classical molecular dynamics (MD) that employ machine learning interatomic potentials (MLIP) offer a favourable scaling of the computational cost, which allow to study large systems over a meaningful time scale. However, its accuracy depends on the quality of the MLIP, which must be trained over a carefully curated database. In this work, we present the machine learning assisted canonical sampling (MLACS) method that combines AIMD with classical MD, and train the MLIP on-the-fly throughout the simulation. We apply this method to study metal hydrides that can be used for solid state storage of hydrogen.

Presenting Author:	Nasim Soltani
Affiliation:	INRS-EMT, Université du Québec, Montreal, Canada
Corresponding Author(s):	Nasim Soltani

Title:	A Regularized Reputation Mechanism for Enhanced Fairness in Federated Learning

Abstract:
Federated Learning (FL) is becoming more popular in the field of machine learning as a decentralized method to protect privacy and avoid over-fitting. However, FL encounters challenges due to the varying quantity and quality of data held by each participant, leading to unequal contributions. Traditional FL treating all participants equally regardless of their input, resulting in unfairness and disadvantaging those who contribute more. To address this issue, our research introduces a reputation-based approach combined with collaborative FL to promote fairness. Additionally, we incorporate advanced techniques like L2 regularization and stochastic gradient descent to improve the model's generalization and mitigate over-fitting.

The proposed reputation formula utilizes validation accuracy metrics to evaluate participants' contributions. These reputations are then refined iteratively to ensure a balanced representation of each participant's involvement.

X= Normalize validation accuracy of each participant
Reputations = sinh((alpha* x [i - 1]) + (x * (1 - alpha)))

To assess fairness, we utilize statistical measures such as Spearman and Pearson correlation, comparing the approach against existing methodologies. Through analysis and experimentation, we demonstrate the effectiveness of the proposed approach in fostering fairness and enhancing model accuracy in FL scenarios.

Presenting Author:	Yasser Salah Eddine Bouchareb
Affiliation:	INRS-EMT, Université du Québec
Corresponding Author(s):	
Title:	Screening binary alloys for CO2 photo capture using GNN

Abstract:
Confronting climate change urgently requires the development of innovative CO2 photocapture technologies. This research project harnesses the synergy of computational chemistry, advanced machine learning, and materials science to fast-track the discovery of effective CO2 capture catalysts. Utilizing Graph Neural Networks (GNNs), we focus on the high-throughput screening and optimization of binary alloys and metal-based materials for photocatalytic CO2 capture. Specifically, we employ tasks from the Open Catalyst Project: Initial State to Relaxed State (IS2RS) to predict the most stable structures after adsorption, Initial State to Relaxed Energy (IS2RE) to estimate the potential energy surfaces, and Structure to Energy and Forces (S2EF) to determine how structural changes affect energy and forces within the catalyst system. These tasks are integral to

evaluating the catalysts' practical efficiency and operational viability under realistic conditions. By deploying deep learning models, our approach efficiently navigates the complexities of material design and streamlines the characterization of these optimized materials. This method not only significantly reduces the time and costs associated with traditional material discovery but also aims to pave the way for the scalable production of cost-effective, high-efficiency catalysts.

Presenting Author:	Jiapeng Zhang
Affiliation:	University of Toronto
Corresponding Author(s):	Chandra Veer Singh
Title:	Dual Model Carbon Engineering in Kilogram-scale Si/C Composites for Stable Lithium Storage

Abstract:

Silicon-carbon composites (Si/C) with multistage structures enable structural integrity during cycling. we have designed the one-step synthesis route for dual-model carbon structure at high temperature, and, based on this, developed a novel pyrolysis device. The controllable combination of two kinds of carbon components is accomplished through the precise adjustment of the pyrolysis temperature. We unravel the dual-model carbon formation mechanism, detailing the cooperative coupling of the nucleation laws of carbon compositions as well as the changes trends in morphology and crystallinity. Combining computational simulations with experiments to investigate the enhancement of lithiation behavior by a dual-model structure. PySi/C's comprehensive electrochemical performance surpasses that of the kilogram-scale Si-based anode reported in recent years.